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ANALYZING NATURAL SYSTEMS:
Analysis for Regional Residuals-Environmental Quality Management

by

Resources for the Future
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16. ABSTRACT

Approaches for analyzing natural systems for regional residuals-environmental quality management (REQM) are presented. System components include land surface runoff, surface receiving water and atmospheric systems. The report identifies and describes the principal approaches and associated analytical techniques used to analyze natural systems, provides detailed summaries of a number of operational natural systems models, indicates the factors that must be taken into account in selecting a model in a given REQM context, describes how to select an appropriate model, and shows how information on modified and new models can be incorporated systematically into an existing framework. The report is intended for individuals in government agencies and the private sector who actually make the analyses to develop strategies for achieving and maintaining environmental quality. A secondary audience consists of those individuals that are involved in making decisions about REQM strategies.

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops management and engineering tools to help pollution control officials achieve water quality goals.

Various planning activities have required that surface waters, groundwater systems, atmospheric systems, and other parts of the natural environment be analyzed to evaluate the effects of human activities on the ambient quality of the respective systems. This report, which presents techniques for analyzing natural systems, is directed to those who must develop strategies for achieving and maintaining an acceptable level of environmental quality.

William T. Donaldson
Acting Director
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Athens, Georgia

Preface

This report had its genesis in various consulting activities and research efforts of the authors at local, regional, state, and federal levels in the United States and abroad. These activities demonstrated the need for, and likely utility of, pulling together and organizing the types of material included herein about analysis for residuals-environmental quality management (REQM). This perception was reinforced by Bower's experience in teaching environmental planning and management over the last decade. The interactions among consulting, research, and teaching helped to shape the effort that resulted in this volume.

The purpose of this report is to bring together information on approaches for analyzing natural systems in the context of analysis for residuals-environmental quality management as that analysis is described in Chapter 1. What is included is not intended to replace or replicate material available in numerous separate publications on analyzing particular natural systems, however those systems are defined. Rather, the purpose is to guide the use of such material in a planning and management context. Therefore, the contents are intended to: (1) identify and describe the principal approaches and associated analytical techniques used to analyze natural systems, (2) provide detailed summaries of a number of operational natural system models, (3) indicate the factors that must be taken into account in selecting a model in a given REQM context, (4) describe how to select an appropriate model, and (5) show how information on modified and new models can be incorporated systematically into an existing framework.

The primary audience for the volume consists of staff members of governmental agencies, enterprises, and consulting firms, the individuals who actually make the analyses to develop strategies for achieving and maintaining ambient environmental quality. This audience is a varied one, ranging from generalist planners with little or no mathematical skills to biologists, ecologists, environmental and sanitary engineers, computer programmers, chemists, economists, political scientists, sociologists, to experienced natural systems modelers. Another component of this audience is comprised of students and teachers concerned, in one way or another, with assessing the impacts of public and private decisions on natural systems.

A secondary audience consists of those individuals and groups that are involved in making decisions about REQM strategies. Examples are heads of executive (line management) agencies, boards of local governments or councils of governments, technical and citizens' advisory committees, legislators and their staffs. In some cases, such as professionals serving on advisory committees, the individuals involved will be as competent technically as the staffs doing the analysis. More common will be the situation in which individuals, while not having a technical background, would still like to know something about how the analysts generated "the numbers." This report will aid in developing that understanding.

The original work for this report was supported by grant number R804528-01-3 from the U.S. Environmental Protection Agency. The original project officer was Charles N. Ehler, who helped to frame the effort. He was succeeded by Harry Torno and Thomas E. Waddell. The continued interest of all three throughout the gestation period is appreciated.

The report was made possible only by the work and contribution of many individuals. Included are those whose names are explicitly attached to the various sections, those whose work elsewhere has been used and cited, and those individuals in federal, state, and local agencies, and in private firms in the United States and abroad, with whom discussions have been held.

We are indebted to reviewers of various drafts. Of particular help were comments from Jo Hinkel, Public Affairs Division, Resources for the Future; Thomas E. Waddell, U.S. Environmental Protection Agency; John Trijonis, Santa Fe Research Corporation, Santa Fe, New Mexico; and R. Gregory Bourne, Environmental Consultant, Atlanta, Georgia.

There were five critical participants in the effort, without whom a final product would not have been possible. Pathana Thananart drafted, redrafted, and reredrafted various diagrams and figures. Martha Bari and Anne Price typed, retyped, and reretyped various drafts and the multitude of tables. Their labors in the residuals pile are much appreciated. Patricia Parker performed, in an outstanding manner, the difficult and complicated task of organizing and preparing the manuscript for publication. Her willingness to undertake this task in the waning hours of the project is especially appreciated. Finally our thanks to Elsa Williams, who designed and produced this Research Paper.

Daniel J. Basta
Blair T. Bower
Washington, D.C.
May 1982

ABSTRACT

Assembled in this report is information on approaches for analyzing natural systems for regional residuals-environmental quality management (REQM). The natural system components analyzed are land surface runoff, surface receiving water, and atmospheric systems. The information is not intended to replace material available in numerous separate publications on analyzing particular natural systems. Rather, the purpose is to guide the use of such material in a residuals planning and management context.

The report (1) identifies and describes the principal approaches and associated analytical techniques used to analyze natural systems, (2) provides detailed summaries of a number of operational natural systems models, (3) indicates the factors that must be taken into account in selecting a model in a given REQM context, (4) describes how to select an appropriate model, and (5) shows how information on modified and new models can be incorporated systematically into an existing framework.

The report is intended for staff members of government agencies, enterprises, and consulting firms--the individuals who actually make the analyses to develop strategies for achieving and maintaining environmental quality. A secondary audience consists of those individuals that are--in one way or another--involved in making decisions about REQM strategies.

This report was submitted in fulfillment of Grant No. R804528-01-3 by Resources for the Future under the sponsorship of the United States Environmental Protection Agency. This report covers the period September 1976 to March 1980, and work was completed as of June 1981.

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Chapter One

INTRODUCTION: ANALYSIS FOR RESIDUALS-ENVIRONMENTAL QUALITY MANAGEMENT (REQM)

Blair T. Bower and Daniel J. Basta

Over the past several decades various models have been developed to analyze natural systems. During the last two decades the development and use of these tools has greatly intensified, primarily in response to the mandated planning requirements of federal, state, and local environmental legislation. The principal legislation that has stimulated development and use of models to analyze natural systems includes: the National Environmental Policy Act (1969); the Water Pollution Control Act Amendments of 1972; the Clean Air Act Amendments of 1977; and related legislation in various states. The various mandated planning activities have required that parts of the natural system, for example, surface water bodies, ground water systems, atmospheric systems, be analyzed to evaluate the impacts of human activities on the ambient quality of the respective systems and to assess the effectiveness of strategies for achieving and maintaining an acceptable level of "quality." In other words, the primary emphasis of natural systems analysis has been within some "management context," however that context has been defined.

A particularly useful framework for describing this overall management context is Residuals-Environmental Quality Management (REQM). The

REQM framework is well-suited to this purpose because it explicitly incorporates all of the activities required to achieve and maintain a specified level of ambient environmental quality. These activities determine the natural systems analyses that are to be undertaken.

The REQM framework has evolved based on research conducted in the Quality of the Environment Division at Resources for the Future. Discussion of some problems relating to analysis for REQM and two case studies are contained in volumes previously published by Resources for the Future. The former is Regional Residuals-Environmental Quality Management Modeling, Blair T. Bower, editor, 1977. The latter two are Environmental Quality Management: An Application to the Lower Delaware Valley, Walter O. Spofford, Jr., Clifford S. Russell, and Robert A. Kelly, 1976; and Analysis for Residuals-Environmental Quality Management: A Case Study of the Ljubljana Area of Yugoslavia, Daniel J. Basta, James L. Lounsbury, and Blair T. Bower, 1978.

This chapter briefly describes the REQM framework and illustrates how natural systems analyses relate to the other analyses and to the activities required for planning and management of environmental quality.

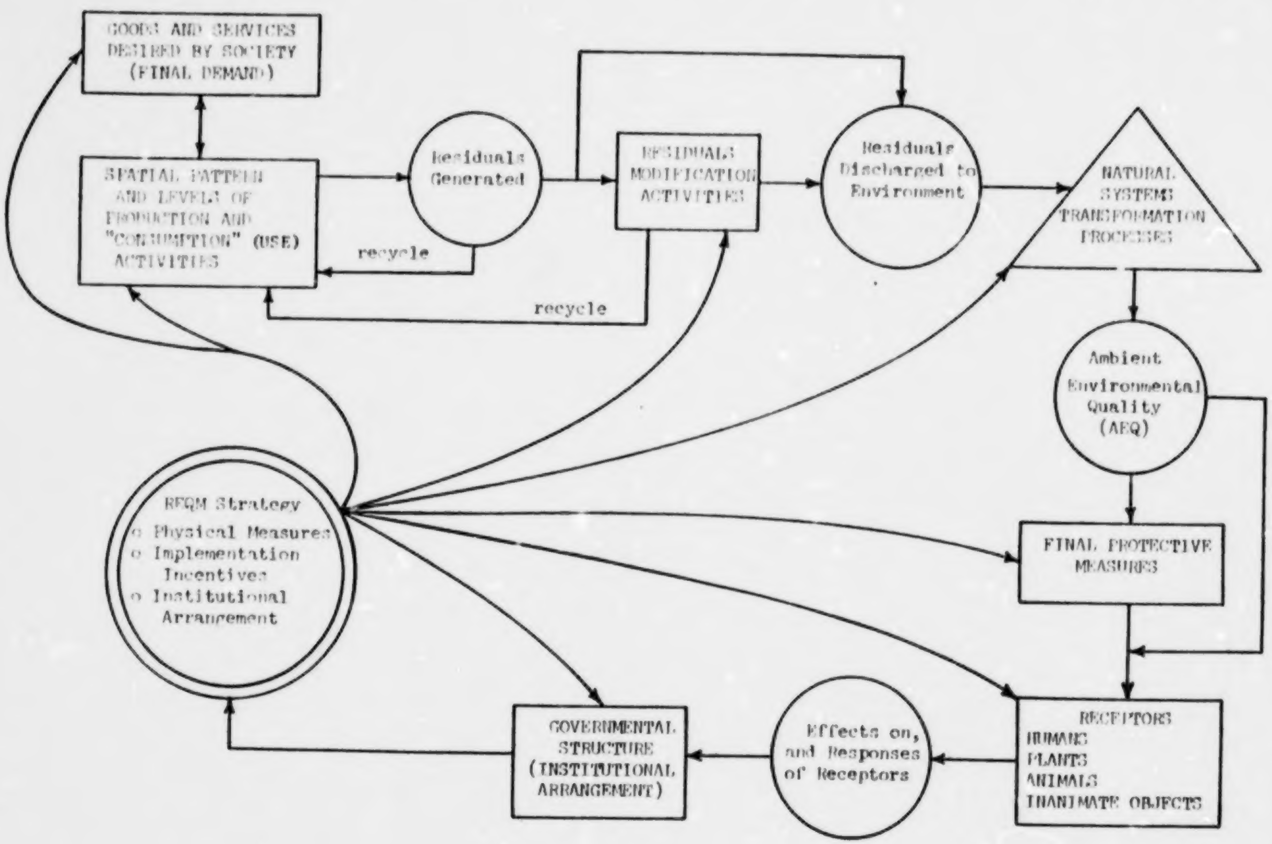
THE REQM CONCEPT

Before proceeding, it is essential to define the term "residuals."[1] This term, as used herein, has a specific meaning, that is, those materials and energy flows which have no value in existing markets or a value less than their costs of collection, transportation, and use in the same or another activity. Thus, a residual is defined in an economic sense. Whether or not a material or energy flow is a residual depends on the relative costs of alternative materials and energy for use in the same or another activity or in other activities. These costs in turn depend on the level of technology in the society and on various governmental policies, both of which change over time. The term residual is used throughout this report rather than such terms as waste, pollutant, or contaminant. An unwanted material or energy flow may or may not accurately be characterized by any one of these terms, depending on the specific material, the environment into which it is discharged, and the effects on environmental quality and subsequent uses of the environment. Not all discharges of unwanted materials or energy into the environment will have adverse impacts on ambient environmental quality; some may in fact have positive impacts. Nor do all changes in ambient environmental quality have adverse effects on receptors.

It is also important to emphasize the interrelationships among the three forms of materials residuals--solid, liquid, and gaseous--because one form of material residual can be transformed into one or more other forms by the addition of materials or energy or both. For example, modification of sewage in a sewage treatment plant results in the generation of a semi-solid residual, sludge, plus various types of liquid residuals. If the sludge is incinerated, a gaseous residual, particulates, is generated. The material and energy inputs required for the modification themselves become residuals. Modification is undertaken under the assumption that the discharge of the modified residual and the discharge of residuals generated in its modification will have fewer adverse impacts than the discharge of the original residual. This may not always be the case. The natural systems analysis to be conducted in any given context must be devised with explicit recognition of these interrelationships.

The concept of an REQM system is illustrated in figure 1-1. Within

Figure 1-1. Concept of a Residuals-Environmental Quality Management (REQM) System


GOODS AND SERVICES DESIRED BY SOCIETY (FINAL DEMAND)
SPATIAL PATTERN AND LEVELS OF PRODUCTION AND "CONSUMPTION" (USE) ACTIVITIES
Residuals Generated
recycle
RESIDUALS MODIFICATION ACTIVITIES
recycle
Residuals Discharged to Environment
NATURAL SYSTEMS TRANSFORMATION PROCESSES
Ambient Environmental Quality (AEQ)
FINAL PROTECTIVE MEASURES
RECEPTORS
HUMANS
PLANTS
ANIMALS
INANIMATE OBJECTS
Effects on, and Responses of Receptors
GOVERNMENTAL STRUCTURE (INSTITUTIONAL ARRANGEMENT)
REQM Strategy
o Physical Measures
o Implementation Incentives
o Institutional Arrangement

any given region (however defined) at a given point in time, there is a spatial distribution of activities: industrial, mining, residential, agricultural, commercial, transportation. This spatial distribution of activities reflects the final demand for goods and services within the region and from outside the region. For each activity there are: (1) alternative combinations of factor inputs and related production technologies to produce the desired goods and services of specified characteristics, with a set of types and quantities of residuals generated associated with each combination; and (2) alternative ways of handling the residuals after generation. Activities as sources of residuals can be classified as: point sources, such as a power plant, a manufacturing plant, a residence; line sources, such as traffic flow on a major street; and dispersed or area sources, such as a logging area or an agricultural operation. Complex point sources, such as large industrial activities, will have multiple stack and nonstack sources discharging to the atmosphere and may have multiple pipes discharging to water bodies. For analysis and management, each stack or pipe may be handled separately, or all stacks and nonstack sources, and all pipes, may be aggregated into a single equivalent stack and a single equivalent pipe, respectively. Similarly, multiple small point sources, such as individual houses in a residential block, may be aggregated for analysis and for some aspects of management.

From each activity some residuals are directly or indirectly discharged into the air, water, and land environments. In the environment these residuals are affected by and may affect various physical, chemical, and biological processes, such as transport, sedimentation, absorption, adsorption, volatilization, decomposition, accumulation. These processes transform the time and spatial patterns of residuals discharges from the various activities into the resulting short-run and long-run time and spatial patterns of ambient environmental quality. What indicators of ambient environmental quality are used at any point in time is a function of: (1) the existing knowledge about the effects of the residuals represented by the indicators; (2) the ability to measure the indicators, that is, the technology of measurement; and (3) the available data.

The resulting time and spatial pattern of ambient environmental quality impinges directly on the receptors--humans, plants, animals, inanimate objects such as structures--or indirectly, as where "final protective measures" are installed between the ambient environment and the receptors. Final protective measures are exemplified by a water intake treatment facility which modifies the quality of water withdrawn from a water body before the water is distributed for use, and by a filter on an air intake. The impacts on the receptors, as perceived by human beings, and the responses of individuals and groups to the perceived damages, provide the stimulus for action. The extent and form of action, as expressed in a selected management strategy, depend on the institutional structure, culture, and value system, and on competing demands for scarce resources for other desired goods and services.

APPLYING THE REQM CONCEPT

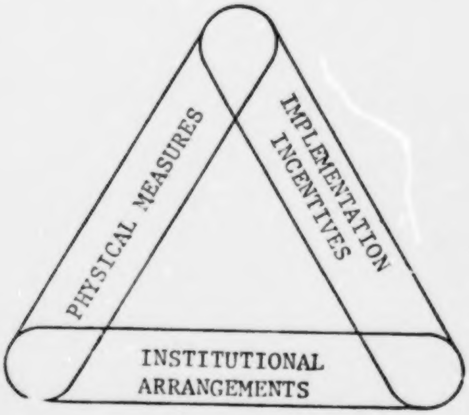
Whatever the geographic focus, the environmental medium (or media) focus (foci), and the institutional context, an explicit set of tasks is required to achieve and maintain a desired level of ambient environmental quality. Operating an effective REQM system requires the following functions: analysis to develop management strategies; planning; legislation; translation of legislation into guidelines and procedures; implementation of guidelines and procedures via incentives imposed on residuals generating activities to induce those activities to install and operate measures for reducing the discharge of residuals or for modifying or making better use of the available assimilative capacity; design, construction, and operation of facilities; monitoring performances by activities and applying sanctions for noncompliance; monitoring of ambient quality; and feedback of information from monitoring into the continuous planning and decision-making functions. It is this total set of functions which yields the desired product of ambient environmental quality.

On a day-to-day basis, REQM takes place primarily at the regional level. The region may be a metropolitan area, a river basin, an airshed, a soil conservation district, an economic region, or some combination of local jurisdictions. Experience indicates that it is less important that the boundaries of the region include all of the residuals dischargers and all those affected by changes in ambient environmental quality than that the boundaries represent some region or area for which there is an institutional arrangement which can be made responsible for REQM. However, where cross-boundary transfers of residuals and their effects are significant, they must be explicitly considered. It is also extremely important to recognize the factors such as national policies iwth respect to taxes, tariffs, imports, and the prices of factor inputs established in national markets affect REQM in a region. Such factors are determined exogenously to the region and comprise part of the context in which REQM takes place; they are major factors which should be--but often have not been--explicitly considered.

A particularly important aspect of applying the REQM concept is the development of management strategies. In REQM the term "strategy" has a specific meaning. An "REQM strategy" is comprised of: (1) the actual physical measures for improving AEQ; (2) the implementation incentives to induce the residuals generators to apply the measures; and (3) the institutional arrangements through which the implementation incentives are applied and the other related activities of REQM are carried out. These three interrelated components are depicted in figure 1-2. Some additional explanation of implementation incentives and institutional arrangements will further illustrate the importance of developing management strategies.

Implementation incentives are the inducements which stimulate the residuals generators and the relevant REQM agencies, for example, metropolitan sewer district, municipal department of public works, to install operate, and maintain the physical measures for improving ambient environmental quality. An implementation incentive can be positive or negative (reward or punishment), direct or indirect, prescriptive or proscriptive.

Figure 1-2. Components of an REQM Strategy



Some implementation incentives can be applied at all levels of government--local, regional, state, national--separately or simultaneously; others are more appropriately applied at a single level. Several characteristics of implementation incentives and their application are important to note.

First, implementation incentives imposed on one residual can have positive or negative impacts on other residuals. For example, an ordinance specifying limits on concentration of particulate discharges from incinerators in buildings may result in closing down some or many of these incinerators with a consequent increase in solid residuals for disposal. The response to an effluent charge on discharge of five-day biochemical oxygen demand may often result in simultaneous reduction in discharge of total suspended solids or phenols.

Second, mixes of implementation incentives can be applied to a given residual generated by an activity. For example, an effluent standard can be coupled with an effluent charge.

Third, many implementation incentives for improving ambient environmental quality are not under the jurisdiction of REQM agencies responsible for managing that quality. Examples include: tax policies such as depletion allowances, severance taxes, capital gains provisions, accelerated depreciation; import restrictions; tariffs, and land use restrictions.

Fourth, some materials are so toxic that their discharge to the environment should simply be prohibited. However, it is no easy task to determine just what materials in what quantities under what conditions are toxic to what species, homo sapiens included. A particular concentration of a material in a body of water may have no adverse effect on some fish species under low or normal temperature conditions, but very adverse effects under high temperatures, or in the presence of some other material, or when dissolved oxygen is low. In some cases, other contributing or intervening variables may affect the response, such as the state of health of the target species. Finally, toxicity is both a short-run and a long-run problem. Concentrations that result in immediate fish kills are obvious; those that result in a buildup in tissues or organs over time, with long-term effects on reproduction and visibility, are not so obvious.

A related problem is the lack of, or incomplete, knowledge of both the effects of the discharge of a residual on ambient environmental quality and the effects on various species from the changes in that quality. Again, both short-run and long-run time frames are involved. The impact of discharges of fluorochlorohydrocarbons on ozone content of the stratosphere is an example. The long-run impact of particulate matter and carbon dioxide discharges on the atmosphere is another.

Finally, the impact of implementation incentives on technological change is important. There relevant question is: Does an implementation incentive bias the selection toward a particular residuals modification technology, or does it stimulate the investigation of the entire range of alternative physical measures in terms of residuals handling technology, altering factor inputs, changing product output characteristics and 'life styles', and changing production technology?

Each implementation incentive has its strengths and weaknesses, so that the implementation incentive(s) chosen in a particular context must be matched to that situation, that is, specific residuals, specific activities, specific physical measures. No one implementation incentive is likely to provide optimal REQM at the local, regional, state, and national scales.

An institutional arrangement is the set of one or more institutions which has or can obtain the legal authority to impose implementation incentives on residuals generators and to carry out the collective tasks of REQM. Factors affecting the choice of institutional arrangement include the spatial dimensions of the REQM problem, available implementation incentives, legal considerations, political considerations, and the cultural values of the society. Consideration of the institutional arrangement is often the weakest link in the development of REQM strategies.

REQUISITE ANALYSES FOR REQM

Whatever the societal and institutional context, making decisions on how to improve ambient environmental quality requires information on the costs and consequences of alternative strategies. The rigorous development of such information is the analysis function of REQM. Planning for REQM is defined as the process of choosing an effective and efficient management strategy, that is, the decision concerning what resources to allocate where, how, and when in order to produce what levels of ambient environmental quality where quality is defined by a set of indicators such as fish biomass, dissolved oxygen concentration, sulfur dioxide concentration, and number of acres devoted to landfills. Analysis, then, is that activity which generates the input to this decision. The output of the analysis consists of the costs and consequences of alternative strategies, criteria for evaluating those strategies, and the results of applying the criteria to the strategies.

Because the nature of environmental quality problems and the resources available for analysis--time, personnel, computational facilities, data--vary from region to region, the degree of sophistication used in the analysis should be "tailored" to the situation. Developing an REQM strategy is not a process which occurs in a vacuum. Rather, the procedure usually involves some region for which one or more environmental quality problems has been perceived or identified or within which questions have been raised. Given such a region, analysis involves the following: (1) the development of models of residuals generation and modification activities, termed "activity models;" (2) the development of models of the processes that affect, and are affected by, the residuals after their discharge into the environmental media, termed "natural systems models;" (3) the specification of an explicit objective function, which includes environmental quality indicators in the function itself, as constraints, or both; (4) the selection of a computational procedure; and (5) the development and application of criteria for evaluating strategies.

For each major residuals-generating activity or group of activities--manufacturing plant, household, municipal incinerator, farm, transport system--an activity model of greater or lesser sophistication is necessary. Such a model: (1) indicates alternative combinations of factor inputs to produce the given outputs of products or services; (2) delineates, for different sets of prices of those factor inputs, the types and quantities of residuals generated per unit of activity, for example, ton of steel produced, kilowatt hour of electrical energy generated, bushel of corn produced, barrel of crude petroleum processed, inhabitant in household; and (3) identifies the various physical measures available for reducing the discharge of residuals into the environment and the costs of various degrees of discharge reudction. Depending on the time and resources available and on the relative importance of the different generators in a given context, activity models may be highly aggregated and simple, or highly disaggregated and complex, and may take the form of mathematical models.

The outputs of the activity models--types and quantities of residuals discharged at specific locations and times--comprise the inputs into the natural systems models, along with the relevant hydrologic, geomorphologic, meteorologic, and pedologic variables such as temperatures, wind velocity, precipitation, soil characteristics, topographic slope, stream channel characteristics, and sunlight. Major types of natural systems models are: (1) physical dispersion models such as for suspended particulates, sulfur dioxide, and total dissolved solids (salinity); (2) physicochemical dispersion models such as for photochemical smog and pesticide movement and modification in ground water aquifers; and (3) biological systems models such as terrestrial and aquatic ecosystem models. Just as for activity models, the time and resources available and the relative importance of the environmental media--in terms of the relevant environmental quality problems--determine the degree of complexity necessary for the natural systems models. For example, a water quality model may consist of a set of simple linear transfer coefficients or it may be a multi-compartment aquatic ecosystem model. Natural systems models tranform the time and spatial pattern of residuals discharges into the environment into the resulting time and spatial pattern of ambient environmental quality as measured by whatever indicators are of interest in the particular situation.

The linkage between activity models and natural systems models merits special emphasis. The activity models must be formulated to provide the data inputs in the proper form for the natural systems models. Conversely, the latter must be formulated in relation to the outputs which the activity models can provide, the available data, and the desired outputs in terms of indicators of ambient environmental quality.

An objective function is a statement of the criterion or the criteria for which the best solution is desired. Constraints are additional factors which must be taken into account in the solution of the problem, factors which limit the range of possible solutions. Criteria can be reflected in the specifications of constraints as well as in the specification of the objective function. Constraints are also part of the decision-making criteria. Specification of an explicit objective function and the accompanying constraints serves to translate the goals or specific objectives of a study into a mathematical or quantitative description of the problem(s).

If damage functions are available which translate changes in ambient environmental quality into monetary damages to receptors, then the objective function can be expressed as maximizing the present value of net benefits, that is, the present value of the time stream of damages reduced minus the present value of the time stream of mitigation costs, over some specified time horizon using the relevant social rate of discount.

However, developing damage functions, that is, determining the relationship between short-run or long-run exposure to the concentration of a residual and physical or physiological effects, and then determining the relationship between those effects and monetary costs, is extraordinarily difficult. In fact, all the necessary damage functions are generally not available to enable use of a net benefit objective function in analysis for REQM. Recourse must then be made to some form of cost minimization objective function, such as minimizing the present value of costs to meet a set of ambient environmental quality standards or limits on discharges, with or without a capital cost or capital plus operation and maintenance cost constraint, and with other constraints, as relevant.

Specification of an explicit objective function and selection of a computational procedure are closely related. The overall computational procedure selected to analyze the effects on ambient environmental quality of alternative REQM strategies and to estimate their costs and consequences is directly dependent on how the objective function for an analysis is specified. The computational procedure selected may or may not involve formal mathematical programming to link activity models and natural systems models. For example, given: (1) a level of output for each activity; (2) the costs of different degrees of individual and collective residuals modification activities; and (3) one or more natural systems models, utilizing a linear programming procedure would yield directly the minimum cost combination of physical measures to achieve the specified ambient environmental quality or to meet specified upper limits on residuals discharges.

Developing and applying criteria for evaluating strategies is a segment of analysis which is frequently given inadequate attention. In REQM, as in all decision-making contexts, criteria must be established by which to choose a preferred strategy. These criteria represent factors which decision makers consider relevant in evaluating strategies. Not only must the criteria be specified, but relative weights must be attached to them.

Although real resource costs represent a major factor in choosing a strategy, these costs do not represent the only criterion. Decision makers in all societies use multiple criteria in making decisions, with the criteria and their relative importance being made more or less explicit. Table 1-1 lists a set of criteria for evaluating REQM strategies. These

Table 1-1. Criteria for Evaluating REQM Strategies

1. Physical Effects
   - a. Reduction in discharge of residual from the activity
   - b. Reduction in total discharge of residual in the region
   - c. Changes in ambient environmental quality and their distributions
   - d. Effects of changes in ambient environmental quality and their distributions
2. Economic Effects and Their Distributions
   - a. Direct benefits
   - b. Direct costs
   - c. Administrative costs
   - d. Indirect costs
3. Administrative Considerations
   - a. Simplicity
   - b. Flexibility
     - (1) Retention of effectiveness under changing conditions
     - (2) Continuous or noncontinuous application
     - (3) Selective or uniform application
4. Timing Considerations
   - a. Years before physical measure is in place and is operating
   - b. Years before impact on ambient environmental quality is realized
5. Political Considerations
   - a. Priority in relation to other environmental quality management problems
   - b. Priority in relation to other societal problems
   - c. Impact on intergovernmental relations, i.e., intercommunal, communal-republic, communal-federal, republic-federal
   - d. Acceptability to public
   - e. Legal difficulties
6. Intermedia and Resource Use Effects
   - a. Intermedia effects: quantities of other residuals generated--gaseous, liquid, solid, noise, thermal
   - b. Resource use effects: net energy use, net land required, net consumptive use of water
7. Accuracy of Estimates
   - a. Physical effects
   - b. Costs

Source: Modified from B.T. Bower, C.N. Ehler, and A. V. Kneese, "Incentives for Managing the Environment," Environmental Science and Technology vol. 11, no. 3, 1977, pp. 250-254.

criteria may be applied to each residual/activity/physical measure/implementation incentive combination, or to each REQM strategy as a whole.

CONCLUDING COMMENTS: NATURAL SYSTEMS ANALYSIS AND REQM

The preceding discussion has described: some of the factors determining residuals generation by activities; the concept of an REQM system; the role of the three environmental media in providing residuals assimilation services, and hence the role of natural systems models; the three components of REQM strategies; and the requisite segments of analysis for REQM. The following are some basic considerations concerning natural systems analysis and the overall "management context" within which they are used, which analysts and managers should explicitly consider.

Strategies for REQM, like decisions in other sectors of the economy, are determined in an institutional milieu. Therefore an important element affecting choice of strategy involves the perceptions of and attitudes toward various aspects of ambient environmental quality. Perceptions and attitudes of individuals and groups are particularly important because all damages from adverse environmental quality and benefits from improving that quality cannot as yet be measured in monetary terms. Thus, to many men and women "on the street," the visible plume from a stack connotes air pollution, even though that plume may be only water vapor. Just what is "clean air" or "clean water" in the minds of individuals, politicians, different groups in society? The "public" perception of indicators of ambient environmental quality is an important consideration in selecting the indicators to be used in the analysis of natural systems.

Ambient environmental quality is a phenomenon which varies over both time and space. It is stochastic because of the basically random nature of meteorologic and hydrologic events affecting assimilative capacity and the random variation in generation and discharge of residuals by activities. More specifically, assimilative capacity varies from location to location within a region and from region to region. The importance of this variation in developing management strategies has been demonstrated by studies which have shown:

a. failure to consider the locations of liquid residuals discharges in a given region can increase by 50 percent or more the costs to achieve a desired level of ambient water quality;

b. failure to consider the locations of gaseous residuals discharges and the affected receptors in an airshed can double at least the costs to achieve a given level of ambient air quality;

c. failure to consider that undesired levels of air quality in many airsheds occur during less than 5 percent of the days, while simultaneously requiring measures to reduce discharges of gaseous residuals 100 percent of the time, can result in quadrupling costs to achieve a given level ambient air quality; and

d. failure to consider variations in assimilative capacity of water bodies among regions, that is, requiring uniform discharge reduction in all regions, will about double national costs to achieve a given level of ambient water quality.[2]

Therefore, analysis for REQM must explicitly include analysis of the stochastic worlds of air, water, and land environments, and of residuals generators, and explicit consideration of space. The operational problems of analyzing natural systems comprise the focus of this report.

CONTENTS OF SUBSEQUENT CHAPTERS

Chapter 2 introduces the analysis of natural systems and provides both a background and a framework for the subsequent three chapters. Appendix B to chapter 2 summarizes the capacity, as of 1979, to model terrestrial ecological systems and describes the requisite attributes of such modeling if it is used in analysis for REQM.

Chapter 3 deals with analyzing residuals generation and discharge from urban and nonurban land surfaces resulting from precipitation and related overland flows of water, phenomena commonly referred to as the "runoff" or "nonpoint" problem.

Chapter 4 concerns the analysis of surface receiving water bodies, including flowing and intermittent streams, rivers of various sizes, lakes, ponds, reservoirs, estuarine systems, and nearshore marine systems.

Chapter 5 deals with analyzing atmospheric systems.

Major types of natural systems models not discussed in this report are ground water models and noise transmission models.

In any attempt to compile and organize materials from multiple sources, some cutoff point in time must be established. That point was 1978-79 for the data on operational natural systems models. Model development is a continuous process in terms of modifications of existing models and development and application of new models. Thus, no compilation is likely to be complete at the time of publication. However, an integral part of this report is a description of how new information on natural systems models can be organized for and assimilated in analysis for REQM.

NOTES

[1] This operational definition is generic, in contrast to the narrow use of the term "residual waste" in the Federal Water Pollution Control Act Amendments of 1972. Section 208(b)(j) of that Act uses "residual waste" to refer only to sludge from wastewater treatment plants. Subsequently, the Environmental Protection Agency broadened the definition of residual waste, as follows: (EPA, 1976, p. 1):

> "Solid, liquid, or sludge substances from man's activities in the urban, agricultural, industrial, and mining environment not discharged to water after collection and necessary treatment. These wastes include, but are not limited to: sludges resulting from water and domestic wastewater treatment, industrial sludges, utility plant sludges, and mining sludges; solids resulting from industrial and agricultural process waste materials and from nonprocess industrial and commercial wastes (e.g., demolition wastes, mine tailings, incinerator residues, dredge spoil, and agricultural waste like crop residues, feedlot wastes and pesticide containers); and liquids resulting from industrial side streams and from agricultural processes."

Given this broader definition, nine "major" categories of sources of residual wastes were identified: (a) wastewater sludge; (b) septage; (c) water treatment residuals; (d) municipal refuse; (e) wastes from combustion and air pollution controls; (f) industrial wastes; (g) feedlot wastes; (h) mine wastes; and (i) dredge spoil (EPA, 1978, p. 2).

The definition of residual herein is broader still; it is essentially the same as the definition used in the Strategic Environmental Assessment System developed under the aegis of the Environmental Protection Agency.

[2] For example, see R. A. Luken, D. J. Basta, E. H. Pechan, The National Residuals Discharge Inventory (Washington, D.C.: National Research Council, January 1976) and available as NTIS Publication No. PB-252-288.

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Chapter 2

INTRODUCTION TO ANALYZING NATURAL SYSTEMS

Daniel J. Basta and David H. Moreau

INTRODUCTION

This chapter contains introductory material on analyzing natural systems and presents an approach for selecting natural systems models (NSMs) in any given residuals-environmental quality management (REQM) context, in relation to specific categories of NSMs discussed in the next three chapters. The first section describes the concept of a natural system as defined in REQM and presents the categories of natural systems discussed in the remainder of the report. The second section identifies and describes the fundamental approaches which in one form or another have been applied to every portion of the natural system. The third section provides operational guidance on how to decide what approach to use in a specific context of analysis and how to choose suitable NSMs from among the populations of models summarized in subsequent chapters. The last section discusses problems associated with applying NSMs and raises some issues in relation to present capacity for analyzing natural systems.

In a region in which analysis for REQM is to be performed, the natural system is defined as the "biosphere," with its component parts or subsystems with which man and his activities interact. Figure 2-1 illustrates this concept, as applied to an illustrative region. The three environmental media--air, land, and water--can be further subdivided for the purpose of analysis. For example, the water subsystem can be divided into surface and subsurface waters, with the former further subdivided by type of surface water body, e.g., lake, stream, estuary. Type of surface water body could be divided still further by other characteristics such as geology and climate.

The state of a natural system varies over time as a result of natural processes and man's activities, the latter exemplified by the discharge of residuals. However, many constituents that are discharged as residuals from man's activities are also generated by, and discharged to natural systems as a result of, natural processes. Some examples are listed in table 2-1.

The state of a natural system, or of any of its component parts, at a given point in time is defined as ambient environmental quality (AEQ). AEQ is measured by indicators such as: the concentration of dissolved oxygen (DO) in a stream; the biomass of fish per cubic meter of water in an estuary; the concentration of sulphur dioxide (SO_2) in the atmosphere over an urban area; the amount of soil eroded from the land surface in a given time period. The indicators used to measure AEQ in any given context are functions of the relevant management problem, available data, and desired AEQ.

Five basic types of processes are at work in natural systems: chemical, biochemical, physical, physicochemical, and ecological. These processes affect the movement, and transformation into other related forms,

Figure 2-1. Illustration of the Concept of Natural Systems in an Hypothetical Region

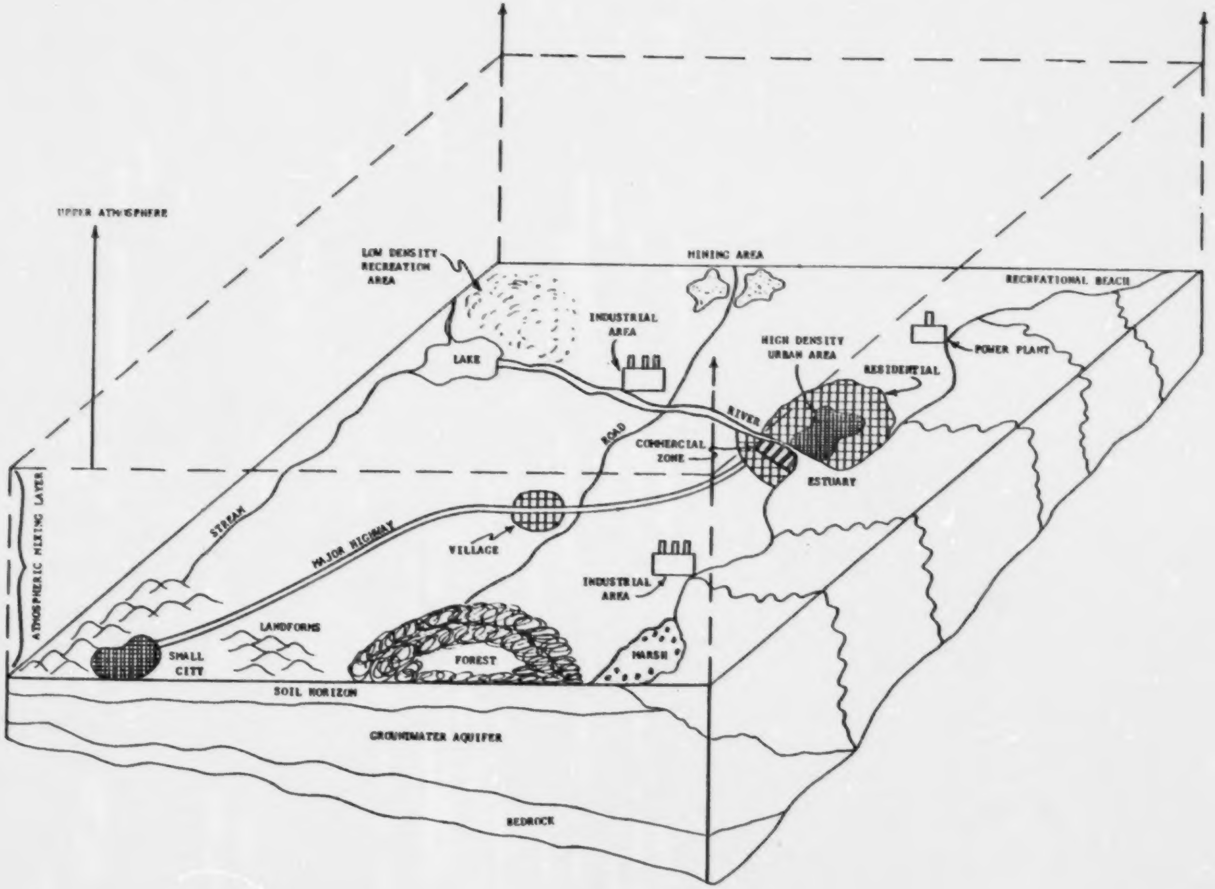

UPPER ATMOSPHERE
ATMOSPHERIC MIXING LAYER
LOW DENSITY RECREATION AREA
MINING AREA
RECREATIONAL BEACH
INDUSTRIAL AREA
LAKE
HIGH DENSITY URBAN AREA
RESIDENTIAL
POWER PLANT
RIVER
ROAD
COMMERCIAL ZONE
ESTUARY
STREAM
MAJOR HIGHWAY
VILLAGE
INDUSTRIAL AREA
LANDFORMS
SMALL CITY
FOREST
MARSH
SOIL HORIZON
GROUNDWATER AQUIFER
BEDROCK

Table 2-1. Examples of Constituents Generated by Natural Processes and Discharged into Natural Systems

Constituent	Natural Process	Environmental Medium
Particulates	wind erosion	air, water
	weathering	air, water
	volcanic action	air, water
	forest and brush fires	air, water
Hydrogen Sulfide (H_2S)	biological decay: oxidation of SO_2 and SO_4 = aerosol in air	air, water
	volcanic action: oxidation of SO_2 and SO_4 = aerosol in air	air, land, and water
Nitrogen Oxides	biological decay: oxidation of NO to NO_2 in air	air, land, and water
Carbon Monoxide	photochemical oxidation of terpenes emitted due to: forest and brush fires, biological decay, plant emanations, yields CO	air, water, land
Hydrocarbons Methane	biological decay of organic materials	land, water
	seepage of natural gas	land
Terpenes	photochemical reaction of terpenes from plant emanation forms aerosols	land
Petroleum	natural seepages	land, water
Dissolved Solids	deposition and concentration of salts due to evaporation, e.g., sea spray, salt springs, saline soils	air, water, land
Heavy Metals	biological action or changes in chemical oxidation state of heavy metal-rich sediments, e.g., geological weathering and erosion	land

of material and energy in natural systems, thereby altering AEQ in both time and space. Chemical processes involve the reaction of two or more compounds with each other to form one or more different compounds. An example of a chemical process in a natural system is the transformation of SO_2 into SO_3 and eventually into H_2SO_4 (sulfuric acid), in the atmosphere. Biochemical processes differ from purely chemical processes in that the transformation is the result of chemical-biological interaction. An example is bacterial decomposition of organic material in a water body where the reaction takes place within a biological organism. Examples of a purely physical process are the movement of particulate matter in the atmosphere by wind currents and the downstream transport of suspended material not subject to decomposition. Physicochemical processes involve the chemistry and physics of molecules as they interact with their surroundings, for example, the adsorption of organic molecules onto solid sediment particles in a stream. Ecological processes involve interactions between or among different species of organisms in the food chain and--for any given organisms or group of organisms--processes such as consumption by prey organisms, growth, mortality, and respiration. The following chapters explain how these processes are taken into account, in lesser or greater detail, in modeling various parts of the natural system.

A natural systems model is defined as a model which translates the time and spatial pattern of residuals discharges into the resulting time and spatial pattern of AEQ or delineates the on-site changes in the state of a natural system as a result of on-site production processes and residuals discharges from the site. The material in this and the following three chapters is not intended to replicate the numerous publications which are available on the various approaches for analyzing in detail parts of natural systems, however defined. Rather, these chapters are intended to: (1) identify and describe the principal approaches and associated analytical techniques presently used to analyze natural systems; (2) provide detailed summaries of a number of operational natural systems models (NSMs) that are currently available; (3) indicate the factors which must be taken into account in selecting an NSM in a given REQM context; and (4) describe how to select an appropriate operational NSM from among those available.

Two attributes are necessary for an NSM to be considered operational. The first is that it has been successfully applied to and verified for at least one application and that it can be used to model another different, but roughly similar, system without extensive internal modification. The second is that sufficient written documentation must be available about the model to enable a potential user to apply the model in a location other than that for which it was verified.

Categories of Natural Systems Models

NSMs have typically been developed by specialized individuals--hydrologists, meteorologists, biologists, engineers, ecologists, limnologists--in a number of different but related fields. Efforts have usually concentrated on one part or subsystem of the natural system. Consequently, there is no one complete and agreed upon classification scheme for categorizing NSMs. However, a classification scheme is important for describing NSMs in relation to REQM, because analysis for REQM may involve the use of several different NSMs, each providing information about a different part of the system.

Five categories of NSMs are delineated herein in relation to analysis for REQM. These are: (1) models of residuals generation and discharge from land surfaces; (2) models of surface receiving waters; (3) models of subsurface waters; (4) models of atmospheric systems;[1] and (5) models of terrestrial ecological systems. Models in the first category produce estimates of residuals generation from land surfaces as a result of the combination of the effects of man's activities on the land surface and natural agents such as rainfall and wind. Examples are the discharge of particulate material from cropland to the atmosphere due to wind action, and the generation and discharge into surface waters of organic material, heavy metals, and suspended solids resulting from precipitation on, and the flow of water over, the land surface. Models in the second, third, and fourth categories produce estimates of the temporal and spatial patterns of AEQ as a result of the discharge of residuals from man's activities into natural systems. Models in the fifth category produce estimates of the state of the natural system itself as a result of endogenous processes at work within the natural system and of external forces imposed on the system, such as effects on soil structure and soil constituents of the combination of pests, application of pesticides, cultivation practices, and crops.

No classification of NSMs is unambiguous. The virtue of the above classification is that it is operational with respect to the ways in which NSMs are integrated into analyses for REQM, including the ways in which different NSMs are linked. Cursory amplification of these definitions is provided here, with detailed discussion reserved for the next three chapters.

Models of residuals generation and discharge from the land surface estimate the temporal and spatial distribution of water and associated materials that run off the land surface and eventually enter receiving waters, as a result of precipitation. NSMs in this category are commonly referred to as "runoff" models. They typically describe the interrelationships among precipitation events (rainfall and snowmelt), surface hydrodynamics, erosion mechanics, and material transport for a given type of surface area. Many of these models also include components which route water flows in channels and pipeline networks before discharge into a receiving water body. Runoff models have been developed to analyze residuals generation and discharge from land surfaces with varying characteristics, as reflected principally by size of surface area (catchment), type of land use, soil characteristics, and frequency, duration, and type of precipitation.

This category of models is operationally divided into two subcategories: models which analyze predominantly urban land surfaces and models which analyze predominantly nonurban land surfaces, such as agricultural and forested lands. Chapter 3 describes this category of NSMs. Appendix A to chapter 3 contains detailed summaries of fourteen operational models of residuals generation and discharge from land surfaces.

Models of surface receiving waters estimate the temporal and spatial distirbution of ambient water quality which results from the discharge of residuals into surface receiving waters. Surface receiving water bodies include perennial and intermittent streams and rivers; lakes, ponds, and reservoirs; estuarine systems; and offshore marine systems. Depending on the context for analysis, the boundaries of the surface receiving water body system under study can encompass a single pond, a section of a reservoir, a few miles of a river, or an entire river basin complete with lakes, tributaries, and mainstream segments. Many receiving water models also include an ecological component which estimates the impact of ambient concentrations of residuals in the water body on various organisms, e.g., plant and animal life. Chapter 4 contains the discussion of surface receiving water models. Appendix A to chapter 4 provides detailed summaries of 27 operational receiving water models.

Models of subsurface waters estimate the flow of water and constituents into, through, and within various subsurface soil and rock strata. The analysis of such natural systems is generally referred to as groundwater modeling. Most models which have been developed in this area are concerned with estimating the flow distribution of water (quantity) in subsurface systems. Very few models currently available address the transport and transformation of constituents in subsurface systems (the quality aspect). Models of subsurface waters are not discussed in this report. However, it is important to indicate that any NSM which involves the transport of water on or over land makes some assumption(s) about, or estimates of, infiltration, percolation, and subsurface flow. Consequently, many of the models presented in the chapters on residuals generation and discharge from land surfaces and on surface receiving waters have components that take into account flows to and from subsurface water systems. However, on their own, none of these components constitutes an operational NSM of subsurface waters, as operational has been defined herein. The present ability to analyze subsurface waters is reflected in Appel and Bredehoeft (1976), Holcomb Research Institute (1977), and Bachmat, et al (1980).

Models of the atmospheric system translate spatial and temporal patterns of residuals discharged into the atmosphere into spatial and temporal patterns of ambient air quality. Such models are also referred to as air quality models. The typical atmospheric system addressed by these models extends vertically from ground level up to and including the atmospheric mixing layer, ordinarily 5,000 to 10,000 feet in altitude, and horizontally encompasses regions on the order of 300 to 500 square miles. Hence, most operational models in this category deal with fairly localized air quality problems, with the possible exception of some models used to analyze photochemical oxidant problems. Models which address the long range transport of residuals in the atmosphere--hundreds of miles--are being developed but were not yet operational, as that term is defined herein, by the end of 1978.[2] Appendix A to chapter 5 contains detailed summaries of thirty-three operational models of the atmospheric system.

Models of terrestrial ecosystems estimate the impacts of intended and unintended alterations of the terrestrial (land) environment on resident plant and animal communities. Major terrestrial ecosystems are classified as: prairies and grasslands; coniferous forests; deciduous forests; deserts; semi-arid brushlands; marshes and swamps. Intended alterations to terrestrial ecosystems occur as a result of man's activities, e.g., constructing buildings, roads, and other structures, or plowing under natural grasslands and growing crops. Unintended alterations are the result of the presence of residuals from man's activities, which residuals result in some change(s) in the natural processes within an ecosystem. An example is the effect on vegetation, and on related organisms in the food chain, of increased soil acidity due to sulfuric acid "washed out" of the atmosphere and deposited on the land surface. Appendix B to this chapter describes the problems of developing terrestrial ecosystem models for use in analysis for REQM. Because most models of terrestrial ecosystems are not operational, as defined herein, detailed summaries of individual models are not presented.

As indicated earlier, NSMs from several of the above model categories could be used in any given REQM analysis, depending on the context. In some cases, outputs from one NSM are inputs into another NSM. One example is when residuals discharges from the land surface, estimated using a "runoff" model, are inputs directly into a receiving water model. Another example is when the quantities of airborne residuals deposited on land or in surface receiving water bodies--as estimated using an ambient air quality model which explicitly considers dry and wet deposition processes--become inputs into a runoff model or a surface receiving water model.

APPROACHES TO ANALYZING NATURAL SYSTEMS

All NSMs involve variations of one of three basic analytical approaches, or a combination of any two or all three of the approaches. This is true regardless of the particular part of the natural system being represented, e.g., surface water body, land area, atmospheric system. These basic approaches are termed: (1) physical (scale) modeling; (2) conservation of mass and energy; and (3) statistical.[3]

Physical (scale) modeling involves building a small-scale physical replica of the natural system of interest, designed to simulate the behavior of the system in a controlled environment. The large physical models of San Francisco Bay and Chesapeake Bay, designed and constructed by the U.S. Corps of Engineers and used to study current patterns, distribution of dissolved solids concentration, and sediment transport and deposition, represent one type of physical modeling. A similar type is exemplified by a scale model of a stack, or set of stacks, for use in wind tunnel experiments. These models are operated to simulate the natural system for some set or sets of conditions, and the effects on AEQ are measured directly, allowing of course for scale effects. Because this report focuses on modeling approaches and models for which arithmetic calculations can be made directly, and because of the relatively limited applicability of physical modeling, no further discussion of physical modeling is presented in this chapter and only minimal discussion is presented in subsequent chapters. However, this does not mean that physical scale modeling is inferior to the other two approaches. To the contrary, in some situations it is superior, and in a few situations it may be the only operational approach.

Models based on the conservation of mass and energy approach attempt to simulate explicitly the processes that transport and transform material and energy in a natural system. Most of these models typically divide a system into a number of segments, e.g., an estuary divided into a number of three-dimensional cells, and then simulate: (1) material and energy flows into each segment or cell; (2) the transformations, if any, which take place within each cell; and (3) the resultant flows out of each cell into other adjacent cells.

Models based on the statistical approach do not explicitly simulate the processes at work in a natural system; they simply provide estimates of the value(s) of the output variable or variables given values of other variables. For example, given a river reach and the objective of estimating the concentration of total dissolved solids (TDS) in that reach, the statistical approach involves two steps. First, one or more variables--the independent variables--are identified on which TDS concentration--the dependent variable--is believed to depend (be a function of). Second, a number of observations of values of all of the variables are made, and some statistical technique is applied, to determine if a statistically significant relationship exists.

This section of the chapter explains the basics of the conservation of mass and energy approach and the statistical approach to analyzing natural systems. At the outset, it is critical to define three characteristics relating to all NSMs: (1) temporal variation; (2) averaging time; and (3) spatial dimensionality. The first refers to how the values of variables in an NSM change over time, i.e., from one time period to the next. The second refers to the time unit over which values of the variables in the NSM are averaged. The third refers to the number of dimensions--one, two, or three--incorporated in an NSM and to the number of segments into which an NSM is divided.

To aid in the explanation, two types of inputs to NSMs are identified, environmental conditions variables and residuals discharge variables. The former refer to such variables as air temperature, wind velocity, wind direction, streamflow, and water temperature. One or more sets of environmental conditions will be of interest to a given REQM analysis. Residuals discharge variables relate to the quantities of various residuals discharged at specific points or over certain areas.

The temporal variation of these variables has two facets: (1) the number of time periods analyzed in an REQM analysis; and (2) the pattern of variation, if any, in values of input variables from one time period to the next time period. Given a series of time periods, ..., t - 1, t, t + 1, ...t + n, where the length of each time period involved can be five minutes, six hours, a day, one month, a quarter of a year, a year, there are three basic types of analyses for REQM with respect to number of time periods analyzed. These are:

(1) a single time period, involving an analysis for a specific set of input conditions for some point or period in time;

(2) two or more time periods, separated by some number of time periods, not necessarily of the same lengths, with no analysis of these intervening periods; and

(3) a number of successive time periods, in which the outputs of the analysis of the first period become the inputs to the analysis of the second period, and so on. (Models incorporating interdependent successive time periods are termed recursive models.)

Thus, an analysis of the first type might involve period t or period t + 10, where t could represent the presnt year, or the seven-day period with the lowest streamflow on record. An analysis of the second type might involve period t, period t + 10, and period t + 25, or period t, t + 1, t + 2, t + 3--representing four seasons of a year--but with no interconnections between any two consecutive periods. An analysis of the third type might involve ten, or twenty, or thirty interconnected periods, e.g., six-hour periods, weeks, years. The first two types are considered steady state analyses, because there are no interconnections between time periods. The third type is considered a nonsteady state analysis, because it involves two or more connected time periods in which the input conditions differ, i.e., the environmental conditions variables, the residuals discharge variables, or both, vary from one time period to the next.

Between a steady state model--in which no variables change for the given time period--and a "pure" nonsteady state model--in which *all* variables, both environmental conditions and residuals discharge variables, change from one time period to the next--there is a continuum. Only a few variables may change from one period to the next, or many, but not all. These "in-between" models might be aptly termed "quasi-nonsteady state" models. For example, in some air quality models environmental conditions variables such as temperature and wind velocity and direction are varied from one time period to the next, while the residuals discharge variables are held constant.

One other distinction with respect to nonsteady state models must be made, namely, that between nonstochastic and stochastic. A nonstochastic model is one in which the variations in each variable from one time period to the next do not include a random component. The term "deterministic" is also used to refer to this type of model. A stochastic model is one in which the variation in one or more of the variables does include a random component. For example, with respect to monthly streamflow, the flow in one month is usually serially correlated with the flow in the previous month (or months), but also reflects a random component.[4] If the set of streamflow inputs used in analyzing the natural system included a random component, the NSM would be a stochastic model. Similarly, if the residuals discharges used as inputs into the NSM included a random component, the NSM would be a stochastic model. Probably there is no completely stochastic model, that is, one in which all variables include a random component.

The above discussion leads to three types of models as defined by these two characteristics: (1) steady state-nonstochastic; (2) nonsteady state-nonstochastic; and (3) nonsteady state-stochastic.

For all NSMs an averaging time must be specified. This is the unit of time for which the values of the variables--environmental conditions, residuals discharges, AEQ indicators--are estimated. For example, dissolved oxygen concentration in a lake can be estimated as an annual average, seasonal average, monthly average, weekly average, and so on. The averaging time chosen in a specific context depends on the management questions to be answered and the NSM used. When episodic conditions are being investigated, for example, with respect to air quality conditions in urban areas, averaging times can be as short as one hour or less. In such a case, a nonsteady state air quality model is used to analyze, hour by hour, a total period of several days, long enough to encompass the episode. This produces estimated values of ambient air quality indicators at hourly intervals throughout the episode.

Spatial dimensionality relates to the number of dimensions--one, two, or three--and number of segments into which a natural system is divided in an NSM. Although any natural system is in reality three-dimensional, simplifying assumptions are often made in order to permit analysis of fewer dimensions rather than all three. The more spatial dimensions explicitly considered in a model, the more complex it is and the greater are its data and computational requirements. Operational NSMs are available which enable analyses of various parts of the natural system in one, two, or three dimensions. Depending on the system to be analyzed and the context, an NSM which considers transport and transformation of residuals in only one or two dimensions may be adequate.[5]

Just as the averaging time for an NSM must be specified, so must the number and size(s) of the spatial or volumetric segments into which the natural system is divided for the analysis. For example, the surface of an urban area 400 miles square can be segmented into 400 one mile square rectangles, or 200 two mile square rectangles, and so on, for the purpose of estimating gaseous residuals discharges. The same urban area can be segmented into ten irregularly sized catchment areas for analyzing urban runoff, or the space above it treated as one volume for analyzing ambient air quality.

Each of these properties is discussed in more detail in the next three chapters in relation to specific categories of NSMs.

Conservation of Mass and Energy Approach to Analyzing Natural Systems

The conservation of mass and energy approach is, in one form or another, the approach used in the majority of NSMs developed to date, and--more important--in the majority of the NSMs currently available. Because this approach is fundamental and common to the next three chapters, it is discussed here in some detail.

The fundamental principles of conservation of mass and conservation of energy comprise the bases for this approach. In their most elementary form these principles assert that mass and energy can neither be created nor destroyed, although they can be altered in form. Given that all residuals are either material (mass) flow or energy flow, these principles provide a set of accounting equations for keeping track of the flow of mass and energy in a natural system. These are the so-called mass balance and energy balance equations. These equations indicate that for any size volume in space--in air, water, or soil--the increase or decrease of mass or energy over any given time interval must be accounted for by either or both: (1) inputs to or outputs from the volume; or (2) transformations in the form of mass or energy within the volume over the given time period. Mass and energy cannot simply disappear. Analyzing a natural system using these principles entails dividing the system into volumes and tracing the movement over time of material and energy flows from volume to volume, using mass and energy balance equations.

Before mass and/or energy balances can be made for a natural system, both the segment or segments to which the balance equations will be applied (spatial dimensionality) and the averaging time over which the balances will be made must be specified. Both spatial dimensionality and averaging time can vary widely, as indicated earlier. At one end of the scale a single space can be defined to cover an entire reservoir or the atmosphere above an entire metropolitan area, e.g., a "lumped" system, or many spaces defined to cover individual segments of a stream up to a few miles in length. A lumped system can be analyzed in relation to one, two, or three dimensions. At the other end of the scale, a natural system may be divided into an almost infinite number of one-dimensional, two-dimensional, or three-dimensional spaces. Figure 2-2 provides some examples of how various natural systems can be sectioned for writing mass/energy balance equations. By writing balance equations for each of the segments and then manipulating the equations simultaneously, the flows of mass (material residuals) and energy (energy residuals) can be traced in one, two, or three dimensions, as may be deemed necessary.[6]

Similarly, the time interval over which the balance equations are written can vary widely. It may be desired to predict changes in AEQ--measured by the amount or concentrations of a specified material in each, or selected, segment(s) into which the system has been divided--over a twenty-year period at one-year intervals, over a period of a few years at monthly intervals, or over a period of several days at hourly intervals. By writing mass/energy balance equations for each successive time interval, the flows of mass and energy can be traced over time in any given segment or for the system under analysis as a whole.

Two points merit emphasis. One, because balance equations are written about gross changes of mass and energy within a given space and inputs and outputs across the boundaries of that space, the equations provide no information about the spatial distribution of mass or energy within the space. Two, similarly, no conclusions can be drawn about the distributions of mass and energy for any time interval less than the interval over which the equations are written.

To illustrate how the principles of conservation of mass and energy are written in mathematical form, consider the three-dimensional box in figure 2-3. Inputs and outputs of mass are considered in only two dimensions.

Figure 2-2. Illustrations of Sectioning Natural Systems for Writing Mass and Energy Balance Equations

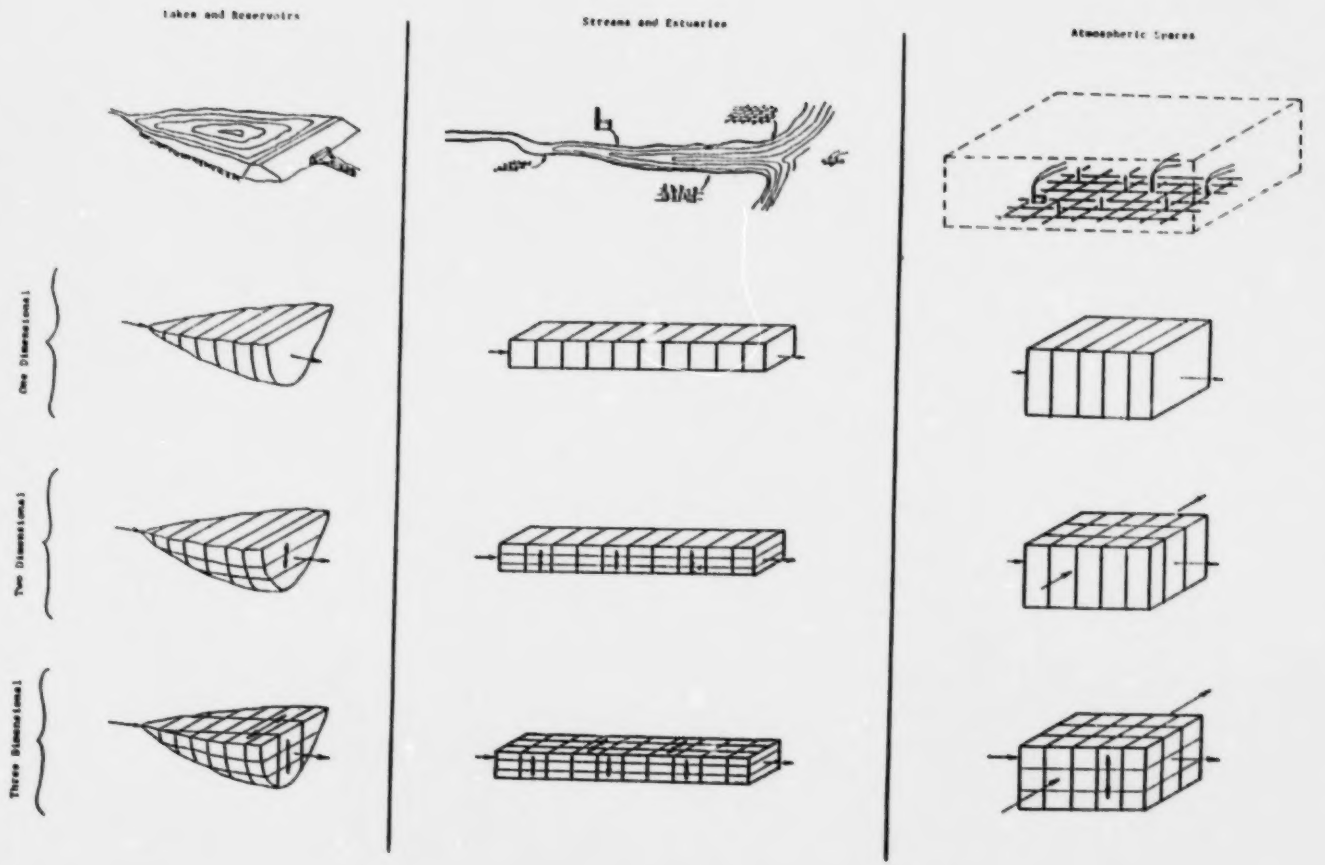
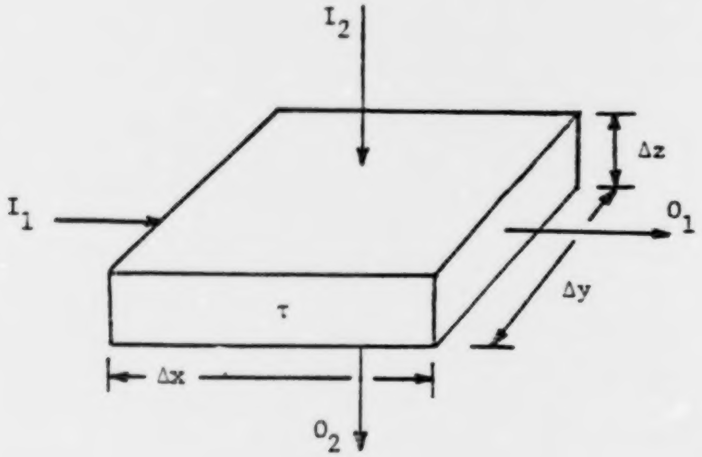

Lakes and Reservoirs
Streams and Estuaries
Atmospheric Spaces
One Dimensional
Two Dimensional
Three Dimensional

Figure 2-3. Unit Volume for Illustrating the Conservation of Mass and Energy Approach to Analyzing Natural Systems



I_1 and I_2 are the inputs of mass of a stated form over some time interval of length Δt; O_1 and O_2 are the outputs; and T is the amount of mass transformed to some other form over that time interval. Then:

$$\Delta M = I_1 + I_2 - O_1 - O_2 \pm T, \tag{2-1}$$

where ΔM is the increase (or decrease) of mass in the box during Δt. Stated more simply: $\Delta M = M_f - M_i$, with M_f being the final amount and M_i the initial amount in the box.

Suppose the box were a space a few feet in depth directly above the land surface of a watershed for which a mass balance equation for stormwater runoff is to be written. When it rains the box receives rainfall as input, R; the box loses water due to infiltration into the ground, L, surface runoff into the adjacent stream, O, and through evaporation, E. If R, L, O, and E represent the amounts of water gained or lost by the box over some time period (Δt), then the increase in water in the box (ΔM)

over time Δt is $M = R - L - Q - E$. In the more general case where there are several inputs, several outputs, and several transformations, equation [2-1] becomes:

[2-2] $$\Delta M = \Sigma I_i - \Sigma O_j + \Sigma \pm T_k \ .$$

(The summation signs indicate that the equation contains more than one term of each kind.)

If it is desirable to express mass and energy balances in terms of rates of change and rates of flow, as is often the case, equation [2-2] can be divided by the time period, Δt, to yield:

[2-3] $$\frac{\Delta M}{\Delta t} = \Sigma \frac{(I_i)}{\Delta t} - \Sigma \frac{(O_j)}{\Delta t} + \Sigma \pm \frac{(T_k)}{\Delta t} \ .$$

The left-hand side, the change of mass in the box divided by the time period, is the average rate of change of mass in the box. It must be recognized that $\frac{\Delta M}{\Delta t}$ is an average rate because the rates over time periods shorter than Δt may vary. Similarly, terms on the right-hand side must be interpreted as average time rates of flow of inputs, outputs, and transformations. Stated in these terms, the mass/energy balance principle is the time rate of increase or decrease of mass or energy in the box must be accounted for by the differences in time rates of inflows, outflows, and transformations, all averaged over a given time period or interval.

Equation [2-3] can also be written in differential form, if Δt is assumed to be an infinitesimally small time interval. The average rates of change would then become instantaneous rates of change, and the equation would be:

$$\frac{dM}{dt} = \Sigma p_i - \Sigma q_j + \Sigma \pm s_k \ ,$$

where p, q, and s are instantaneous rates of inflow, outflow, and transformations, respectively.

The foregoing discussion has set forth the basic principles of conservation of mass and energy and indicated how these principles are used to analyze natural systems. Equations representing conservation of energy are analogous to those presented for conservation of mass. However, the general mass and energy balance equations stated above are gross simplifications of reality. Rarely are these simple equations sufficient for predicting spatial and temporal patterns of mass and energy levels in natural systems. Various expressions which explain the factors which govern the rates of inflow, outflow, and transformations must be incorporated into the general equations. Depending on the individual natural system being analyzed, these rates are controlled by various natural processes operating independently or jointly. Typical processes include: gas transfer; heat transfer; fluid movement; advection and diffusion of materials in water and air; sedimentation of solid materials; and chemical, biological, and photochemical reactions.

Of all the processes which govern rates of inflow and outflow, the mass transport processes of advection and diffusion are important in most problem settings. Almost all NSMs based on the conservation of mass and energy approach--runoff models, receiving water models, and air quality models--explicitly take into account these two processes. Therefore, an explanation of how advection and diffusion are incorporated in the balance equations of the conservation of mass and energy approach is presented next. Explanations of how other processes are incorporated into the balance equations are provided in the next three chapters, where relevant.

As will be indicated, it is simply not possible to account explicitly for some of the processes which govern rates of change in natural systems, given present knowledge.

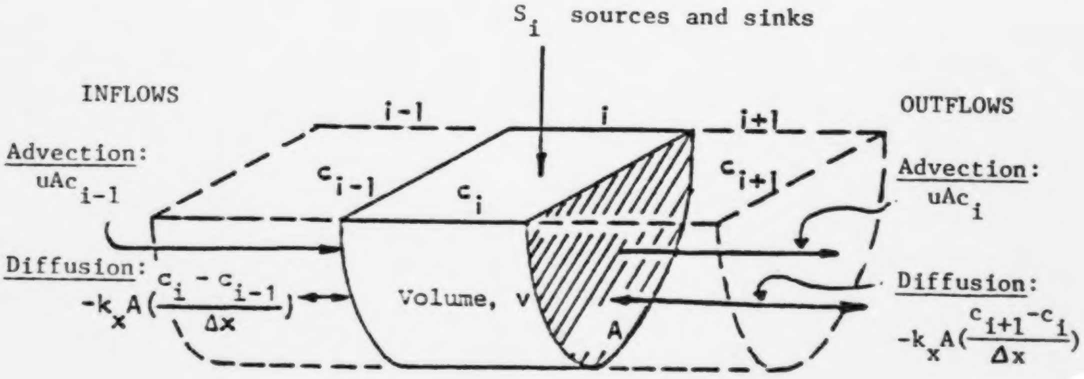
Advection and Diffusion

Advection is the process by which materials and energy are transported through space by the movement of the fluid medium within which they are either suspended or dissolved. Both air and water are fluid media. Advective transport simply means that materials and energy are carried along with water and air currents at the same velocity as the currents. For example, for the three-dimensional box in figure 2-3 (page 47), given: cross-section area, A, concentration, c, of a material in a fluid about to enter the box at the cross-section, and the velocity, u, of the fluid at the same cross-section, the rate of flow of mass entering the box through the cross-section is simply equal to $c \cdot u \cdot A$.

Diffusion is a more complicated mass transport process than advection because there are several different kinds of diffusion which may occur simultaneously in any given natural system. Types of diffusion include: Brownian motion of molecules; eddy diffusion due to the swirling motion of a fluid; and turbulent mixing due to random motion of microscopic particles. Whatever the type, the result of diffusion is eventually to distribute materials (or energy) evenly throughout a body of water or air. The tendency is for mass or energy within fluids to move from regions of higher concentrations to regions of lower concentrations. In most NSMs, the rate of mass or energy transfer due to diffusion is assumed to be proportional to the concentration gradient, that is, proportional to the change in concentration, c, going from a region of high concentration to a region of low concentration, over a specified distance, Δx. Mathematically, the rate of mass transfer due to diffusion is expressed as, $-kA \frac{\Delta c}{\Delta x}$, where A is the cross-sectional area of a three-dimensional box into which mass transfer is to be estimated, and k is a constant of proportionality called a diffusivity coefficient. The negative sign indicates transport in the direction of the negative gradient.

To illustrate how advection and diffusion are incorporated into a mass balance equation, consider the discharge into an estuary of a nonreactive or conservative residual, i.e., one which does not change form in the fluid medium. Assume that advection and diffusion are the primary mass transfer processes, and that the problem is defined in terms of transport in one direction only, downstream. To write mass balance equations, the estuary is divided into a number of sections, i = 1, 2, ..., n, as shown in figure 2-2 (page 46). To simplify the problem, it is further assumed that complete mixing takes place in each section of the estuary. This set of assumptions defines a one-dimensional estuary, as shown below.

Figure 2-4. Typical Section for a One-Dimensional Estuary


S_i sources and sinks
INFLOWS
i-1
i
i+1
OUTFLOWS
Advection:
uAc_{i-1}
c_{i-1}
c_i
c_{i+1}
Advection:
uAc_i
Diffusion:
$-k_x A(\frac{c_i - c_{i-1}}{\Delta x})$
Volume, v
A
Diffusion:
$-k_x A(\frac{c_{i+1} - c_i}{\Delta x})$

For each section of the estuary, the following mass balance equation can be written:

$$\begin{aligned}\begin{array}{r}\text{Average rate}\\\text{of change}\\\text{of mass}\end{array} &= \left(\begin{array}{c}\text{Average rate of inflow}\\\text{due to advection}\end{array}\right) - \left(\begin{array}{c}\text{Average rate of outflow}\\\text{due to advection}\end{array}\right)\\ &+ \left(\begin{array}{c}\text{Average rate of inflow}\\\text{due to diffusion}\end{array}\right) - \left(\begin{array}{c}\text{Average rate of outflow}\\\text{due to diffusion}\end{array}\right)\\ &\pm \left(\begin{array}{c}\text{Sources and}\\\text{Sinks}\end{array}\right) .\end{aligned} \tag*{[2-4]}$$

The amount (mass) of the material, M, of interest in any section of the estuary, at any point in time, is equal to the product of the volume of water, v, times the concentration, c, mass per unit volume of the material in the section. If the volume of water in each section is assumed to be constant over time, i.e., steady-state flow conditions are assumed, then the change in the amount of material in any sector over some time interval can only be accounted for by a change in concentration. Hence, for the ith section, the change in mass of the material for a given time interval can be written as

$$M_i^{j+1} - M_i^j = v_i \, (c_i^{j+1} - c_i^j) .$$

Because it is assumed that each section is completely mixed, the outflow due to advection from each section is $u\,A\,c_i$, where u and A are the velocity of flow and cross-sectional area for the ith section. The outflow from an upstream segment becomes the inflow to the next downstream segment. The inflow of mass due to diffusion is given by, $-k_x A \left(\frac{c_i - c_{i-1}}{\Delta x}\right)$, and outflow by, $-k_x A \left(\frac{c_{i+1} - c_i}{\Delta x}\right)$. Substituting these expressions into equation [2-4] yields:

$$\frac{v(c_i^{j+1} - c_i^j)}{\Delta t} = uAc_{i-1} - uAc_i - \frac{k_x A}{\Delta x}(c_i - c_{i=1}) + \frac{k_x A}{\Delta x}(c_{i+1} - c_i) \pm S_i \,, \tag{2-5}$$

where S_i represents sources and sinks of material in each section.

The system of equations represented by equation [2-5] constitutes a set of linear equations for estimating the concentration of the material in each section of the estuary. Note that the rate variables on the right-hand side of equation [2-5] are interpreted as average values. If initial concentrations for each section and at the upstream and downstream boundaries of the estuary are specified, then a concentration profile--concentrations in each section into which the estuary has been divided--can be estimated by iterative solution of the system of equations.

Equation [2-5] represents the general nondifferential form of the conservation of mass equation for one-dimensional flow in the x-direction, based on the processes of advection and diffusion. Depending on the natural system to which it is applied, and the methods used to estimate the velocities in any given section, the diffusivity coefficients and exogenous inputs into each section will vary.

The above explanation of how advection and diffusion are incorporated in mass balance equations for analyzing natural systems was illustrated by a very simple example. The formulation for analysis of energy balances is analogous to that presented above for mass balances. In actual applications to NSMs, the mass balance equations are more likely to be in differential form, rather than in the simple algebraic form shown above. Therefore, the next section briefly describes the general differential form of the conservation of mass and energy approach as applied in NSMs. No derivation of the differential form is provided; the derivation can be found in many references, such as Dailey and Harleman (1966) and Bird, Steward, and Lightfoot (1960).

The Differential Form of the Conservation of Mass and Energy Approach to Analyzing Natural Systems

In order to convert equation [2-5] into differential form: (1) the intervals Δt and Δx are reduced to infinitesimally small values dt and dx; (2) the instantaneous rate of change in concentration at any point in time is given as the partial derivative $\frac{\partial c}{\partial t}$; and (3) the instantaneous rate of change in concentration with respect to change in location is given as the partial derivative $\frac{\partial c}{\partial x}$. After various manipulations similar to those described in the previous section, the differential form in one dimension is:

$$\frac{\partial c}{\partial t} = - u\frac{\partial c}{\partial x} + k_x\frac{\partial^2 c}{\partial x^2} \pm S \; . \tag{2-6}$$

Following the same reasoning, a three-dimensional mass balance equation which includes advection and diffusion can be derived by extending the one-dimensional equation. For the three-dimensional case where advection and diffusion occur in the x, y, and z directions, the mass balance equation--assuming homogeneous diffusion in all three directions--is:

$$\begin{aligned} \frac{\partial c}{\partial t} &= - u_x \frac{\partial c}{\partial x} - u_y \frac{\partial c}{\partial y} - u_z \frac{\partial c}{\partial z} \\ &\quad + k_x\frac{\partial^2 c}{\partial x^2} + k_y\frac{\partial^2 c}{\partial y^2} + k_z\frac{\partial^2 c}{\partial z^2} \pm S \; . \end{aligned} \tag{2-7}$$

Equation [2-7] is the basic equation behind all NSMs based on the conservation of mass and energy approach. Depending on the natural system and on the processes which are assumed to predominate, the solution to this equation can take various forms. Some of the assumptions and related forms of the conservation of mass equations are discussed in the next three chapters.

The only two ways in which the differential equations [2-6] and [2-7] can be solved are analytical integration and numerical integration. Analytical integration is when an expression for the rate of change of a variable--a differential equation--is transformed using calculus methods to yield an algebraic equation which, when solved, will give the value of the variable. Analytical solutions to the conservation of mass equation are possible, given certain assumptions about such factors as: boundary conditions; flow conditions; the relative strengths of advective movement of material in different directions; how exogenous inputs of material, e.g., residuals discharges, enter each section of the natural system. One of the most popular of these analytical solutions is the Gaussian form. This form has had considerable application, particularly in modeling ambient air quality. (The Gaussian form is discussed in more detail in chapter 5.) However, it is important to emphasize that distortions introduced by many of the simplifying assumptions required to enable analytical integration of the differential form of the conservation of mass and energy equations are unacceptable in many REQM problem contexts. Therefore, methods of approximation are frequently employed to solve the equations, eliminating the need for at least some of the simplifying assumptions.

Numerical integration is when the differential form of the conservation of mass and energy equation is solved by some approximation methods. It consists essentially of obtaining numerical values of the unknown integral (solution to the integration of the differential equation) at several spatial locations and/or for several time periods. Then--by fitting linear or higher order curves through these points--the derivatives of the differential equation are estimated from the derivatives of the curves.

Numerical integration has become increasingly popular in recent years for analyzing natural systems because it enables solving complicated equations which previously were not solvable. Thus, numerical integration is used in the majority of operational NSMs currently (1978) available, particularly for NSMs of surface receiving waters and atmospheric systems.

Various methods of numerical integration are available. The finite difference method, and variations thereof, is by far the most frequently employed. For additional explanation of numerical integration, see Salvadori and Baron (1961) and Tracor, Inc. (1971).

Whether models based on the conservation of mass and energy approach are analytically or numerically integrated, a computer is almost always necessary. Some additional discussion of analytically and numerically integrated NSMs, and related references are provided in the next three chapters.

Concluding Comments on Conservation of Mass and Energy Approach

The foregoing discussion has described the principles of the conservation of mass and energy approach to analyzing natural systems primarily from the perspective of tracing the movement of mass and energy in air and water via advection and diffusion. Indeed, there are numerous other applications of these principles in analyzing natural systems, such as in tracing linkages among species in the food chain in ecological modeling. Thus, regardless of the natural systems being analyzed and the problem context within which the approach is applied, the development of mass and energy balance equations will be analogous to the above presentation. In almost all cases balance equations will be expressed in terms of rates of change--differentials--and will require simultaneous or sequential solution, regardless of whether the sections for which the equations are written represent volumes of water or groups of organisms residing over some land area. In the latter case, rates of change could refer to uptake of certain nutrients, predation on other species and on the species of interest, and production of waste products by various species.

Statistical Approach to Analyzing Natural Systems

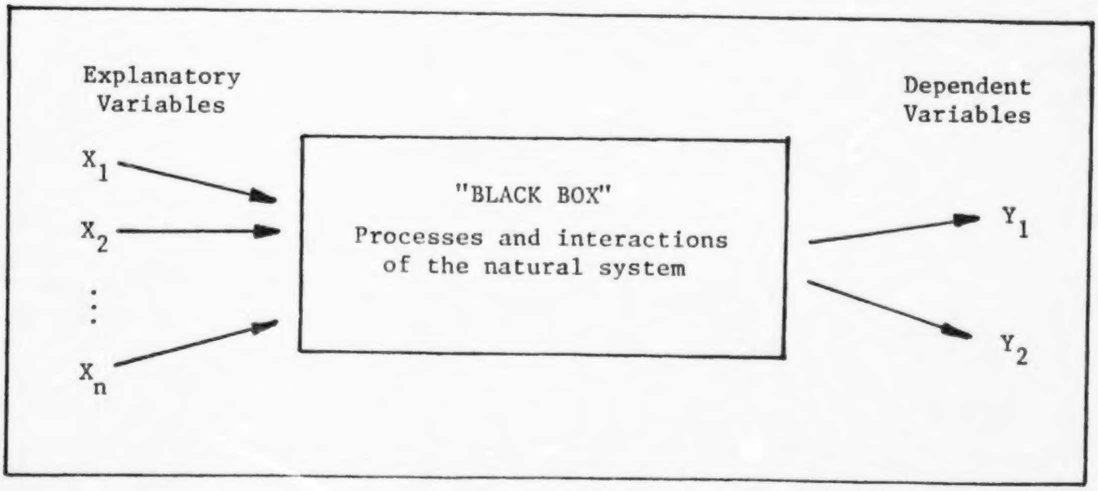
The statistical approach has long been used in analyzing natural systems. Various statistical methods have been applied to a broad range of problems and in varied contexts. The essence of the approach is the determination of a statistically significant relationship between a dependent variable and a number of independent variables. The dependent variable is an indicator of AEQ and the independent variables must include residuals discharge variables.

The approach is conceptually simple. For a natural system being analyzed, first the relevant variables are posited, based on knowledge of the physical, chemical, and biological phenomena involved. That is, variables which are believed to affect the dependent variable of interest are posited. Second, one or more structural forms of the relationship between the independent variables and the dependent variable are posited. Third, a set of data with values of each of the variables is obtained. These observations can be taken over time, in which case they are termed time-series data, or can represent a sample of individuals, groups of individuals, geographical areas, or even objects, in which case they are termed cross-sectional data.

As noted previously, the statistical approach does not explicitly consider the various processes operating in the natural system, e.g., various physical, chemical, and biological processes and interactions among components of the natural system. The statistical approach views the natural system as a "black box"--as shown in figure 2-5--with some inputs (the independent variables) and some outputs (the dependent variables). The "internal workings" of the black box remain unknown and unspecified.

What is implied in figure 2-5 is that, in some cases, several dependent variables are functions of the same independent variables. That is, $Y_1 = f(X_1, X_2, \ldots, X_n)$ and $Y_2 = f(X_1, X_2, \ldots, X_n)$. For example, BOD and DO concentrations in a given reach of a stream are functions of the same variables. The relationships are of course developed separately.

Figure 2-5. Representation of the "Black Box" Concept in the Statistical Approach to Analyzing Natural Systems


Explanatory Variables
Dependent Variables
X1
X2
Xn
"BLACK BOX"
Processes and interactions of the natural system
Y1
Y2

Regression analysis is the most common statistical method used in developing statistical NSMs.[7] Common structural forms of an hypothesized relationship are linear, semi-log, and log-log, e.g.:

[2-8a] $$Y = \alpha + B_1X_1 + B_2X_2 + \ldots + B_nX_n + E;$$

[2-8b] $$\log Y = \alpha + B_1X_1 + B_2X_2 + \ldots + B_nX_n + E;$$

[2-8c] $$\log Y = \alpha + B_1\log X_1 + B_2\log X_2 + \ldots + B_n\log X_n + E\ .$$

Y represents the dependent variable(s), $X_1 \ldots X_n$ the independent variables, E a random disturbance term, α a constant, and $B_1 \ldots B_n$ coefficients to be estimated. Statistically significant coefficients indicate the relative degrees to which the various independent variables explain variations in the value of the dependent variable. "Statistically significant" is usually defined in terms of a probability level. For instance, if a coefficient is significant at the 95 percent level, then the inference may be made that there is only a 5 percent chance that the coefficient could be of such magnitude by chance.

Various procedures are available for solving a regression equation, and computational packages for obtaining solutions are available for almost any computer system. These packages usually compute "test statistics" which assess statistical significance for each variable and for the equation as a whole.

Statistical methods are also used in developing inputs for the conservation of mass and energy approach to analyzing natural systems. Many of the environmental conditions and residuals discharge variables are stochastic; hence, using statistically determined probability distributions of their values for inputs is appropriate. Examples of such use are the estimation of diffusivity coefficients for some receiving water models and wind field coefficients in some air quality models. The results of such applications are not operational NSMs as defined herein, because the output is not some indicator of AEQ and because no residuals discharge variables are involved. Thus, equation [2-8] would be considered an NSM only if the dependent variable, Y, were, for example, ambient concentration of SO_2 or quantity of runoff from the land surface. If Y represented a diffusivity coefficient, then equation [2-8] would not be an NSM.

NSMs based on the statistical approach cannot be transferred intact to other regions when such NSMs contain coefficients empirically derived from a particular area. These coefficients are functions of the geologic, hydrologic, hydraulic, meteorological conditions in the area and the spatial pattern of residuals discharges in the area. However, a statistically significant relationship found in a given area would suggest both relevant variables and a structural form to try in another area, for the same dependent variable(s). Examples include the application of the Universal Soil Loss Equation for estimating gross soil erosion from agricultural areas and regression analysis applied to eutrophication in lakes. The former is discussed in chapter 3, the latter in chapter 4.

The statistical approach to analyzing natural systems has the problems of all statistical analysis, e.g., specification and multicollinearity. Where time series data are used, autocorrelation may be a problem. These problems are discussed, for example, in Cooley and Lohnes (1966) and Miller and Freund (1965). However, the most important limitation is that the statistical relationship developed from a given set of data for some natural system reflects the particular spatial arrangement and levels of residuals discharging activities and natural system processes which existed when the data were collected. For any markedly different spatial patterns, processes, levels, new data would have to be obtained and a new statistical relationship developed. As a result of these problems and limitations, the statistical approach to analyzing natural systems has been used primarily where: (1) only a "first cut" crude analysis is required; or (2) no NSM based on the conservation of mass and energy approach is available or can be developed, either because of scarce resources or because of the complexity of the natural system to be analyzed.

SETTING UP THE NATURAL SYSTEMS ANALYSIS

In any REQM analysis, one or more natural systems must be analyzed. The analysis may take the form of a "back of the envelope calculation" or a sophisticated, numerically integrated, multicompartmental, conservation of mass and energy ecological model. The factors determining the scope and the type(s) of natural systems analysis undertaken include: the questions to be answered; the residuals of concern; the conditions of relevant natural systems measured in terms of AEQ indicators; available analytical resources; and the relative importance and characteristics of residuals generating activities. Therefore, setting up the natural systems analysis requires careful consideration of the other REQM analysis segments: estimating alternative levels and spatial patterns of activities; analyzing activities; formulating and analyzing strategies; and evaluating strategies.

This section discusses setting up the natural systems analysis portion of an REQM analysis. The presumption is that a logical sequence of steps can be followed to ascertain what natural systems analysis is to be undertaken, regardless of the context. The section sets forth this sequence and indicates how the material about specific categories of NSMs contained in the remaining chapters of this report can be used for this purpose.

Before beginning to consider the scope and types of natural systems analyses required, certain analysis conditions must be specified. These conditions are specified early in the process of setting up an REQM analysis. At the very least, preliminary specification of: (1) residuals of concern; (2) the questions to be answered and a translation of them into specific information to be generated on AEQ and on related REQM costs; (3) relevant time periods for the analysis; and (4) boundaries of the region to be studied, are necessary to begin the determination of what natural systems analysis(es) is (are) required.

Step 1: Identify AEQ Problems

Given a specification of the analysis conditions, the first step is to make a preliminary identification of the environmental media and the relevant characteristics thereof that are affected by discharges of the residuals of concern. This would be accomplished without actually carrying out formal modeling analysis per se, but would be based on experience with and knowledge of the pathways, movements, and related effects of those residuals when discharged to the environment. For example, if eutrophication were identified or suspected as a major problem in a surface receiving water body, preliminary inferences could be drawn about the natural systems analyses required. First, because it is known that in most cases nutrients--nitrogen, N, and phosphorus, P, compounds--are controlling factors in eutrophication, and because large quantities of N and P can enter receiving waters in runoff from land surfaces, some analysis of residuals generation on the land surfaces in the region is likely to be required. Second, any receiving water NSM used would have to consider explicitly N and P inputs. The purpose of this first step is to make a preliminary identification of the categories and characteristics of NSMs that might provide the required information.

Step 2: Perform Preliminary Analysis

The second step is to perform a preliminary analysis of the natural systems or subsystems identified above as being relevant, given whatever data are available with respect to residuals discharge variables, environmental conditions variables, and AEQ variables. The purposes of a preliminary analysis are to determine: (1) if the right questions have been asked regarding the natural system; (2) if all of the important residuals have been identified with respect to impacts on the AEQ indicators of interest; (3) the relative importance of various point and nonpoint sources of residuals; (4) the potential importance of intermedia transfers; and (5) additional characteristics of the AEQ problem which will help to determine which approaches to use to analyze the relevant natural systems.

Preliminary analysis employs relatively simple analytical methods, requires little data, and can usually be accomplished with the aid of a desk-top calculator or slide rule. Such methods for analyzing natural systems exist, as do various simplified NSMs, which can be used in the preliminary analysis. For example, simplified mass balance equations are frequently used to make preliminary analyses in a variety of contexts. The Streeter-Phelps relationship for predicting biochemical oxygen demand

(BOD) and dissolved oxygen (DO) interactions in streams and rivers can be implemented on a desk-top calculator.

Simple methods for analyzing natural systems are not discussed in this report. However, several relatively simple NSMs for use in preliminary analysis of runoff problems are identified and described in chapter 3. Also, some of the models summarized in the chapters on surface receiving waters and atmospheric systems qualify as relatively simple models and have been used for preliminary or "first cut" analyses. Appendix A to this chapter contains a list of references on relatively simple methods for analyzing natural systems and a list of those models summarized in the next three chapters which are applicable for preliminary analysis.

The extent to which a preliminary analysis is required depends on the context. In many regions natural systems analyses of one form or another have already been carried out. Any additional analysis should build on previous work. Enough might be known so that a preliminary analysis might not be required. On the other hand, there are regions where little or no analysis of natural systems has been done. Further, even where analyses have been made, newly recognized problems and new residuals of concern are likely to mean that the preliminary analysis step is essential.

Step 3: Specify Level of Complexity

Given the results of the preliminary analysis, the third step is to specify in detail the level of complexity necessary to generate the requisite information about each part of the natural system to be analyzed. Level of complexity is defined in terms of: (1) the time interval(s) of analysis, i.e., hourly, daily, monthly, seasonally, annually; (2) spatial aggregations, i.e., number of grid areas, stream reaches, lake layers; (3) constituent/species aggregations to be explicitly considered, i.e., forms of nitrogen, number of fish species; and (4) the specific physical, chemical, and biological processes to be explicitly considered. This specification process defines the characteristics which are used to identify an appropriate NSM or appropriate NSMs to be used.

Step 4: Determine Feasibility

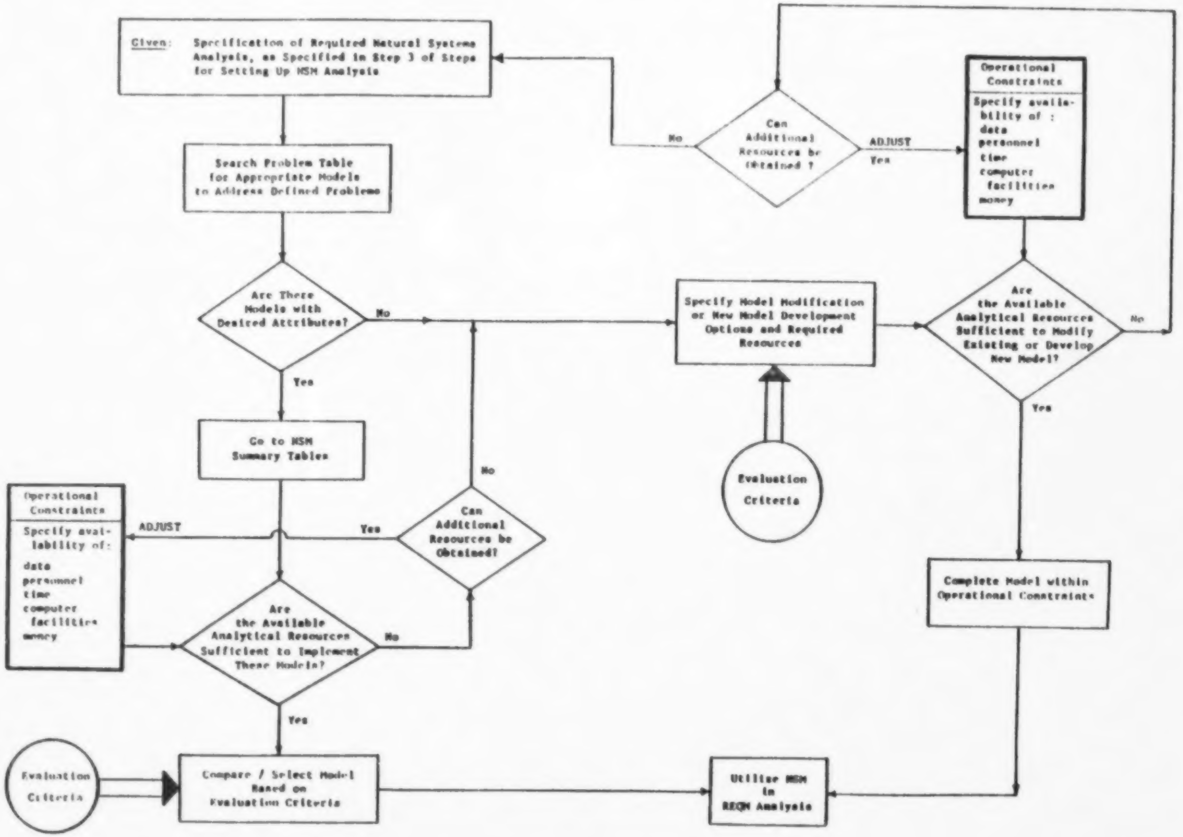
The fourth step is to determine the feasibility of carrying out the natural systems analysis specified in step 3. If, for any category of natural systems analysis, at least one operational NSM can be identified which is able to generate the information required, incorporate the level of detail specified, and be executed within the operational constraints, then the natural systems analysis as specified is considered feasible. If no operationsl NSMs can be identified for a given category of natural systems analysis, the required analysis might be feasible if an existing model could be modified, calibrated, and verified, or a new model could be developed, calibrated, and verified, within the operational constraints. If neither of these procedures is feasible, two basic options remain. One, the operational constraints on the natural systems analysis can be modified, i.e., more analytical resources provided. Two, if the available analytical resources cannot be increased, the specifications for the natural systems analysis must be modified. That is, less information--in scope, detail, or both--would be required about the natural systems and the effects of residuals discharges on them.

Assessing the available data is a critical task in step 4. In this connection, what is required is a detailed enumeration of: (1) available data which can be used without modification, i.e., data which have the requisite detail and accuracy; (2) available data which must be modified before use, the details of the required modification, and the analytical resources required to execute the modifications; and (3) additional data which would have to be obtained in order to use the specified NSM(s) and the resources required to obtain the data.[8] If the data ready for use are insufficient or cannot be modified, and additional data cannot be obtained to enable use of the specified NSM(s) in the time frame for the REQM analysis, then the specified NSM is, or NSMs are, infeasible.

Further amplification of step 4 is merited. In order to identify operational NSMs which might be feasible in a given context, each of chapters 3, 4, and 5 contains a section on selecting an appropriate NSM. These sections are all organized in a similar format. They contain five elements: (1) a list of both operational and nonoperational NSMs referred to as a population table; (2) a table which relates problem characteristics to the operational NSMs included in the population table, referred to as a problem table; (3) a flow diagram which indicates how to select an appropriate NSM using material included in the chapter, referred to as a selection procedure, analogous to that shown in figure 2-6; (4) a discussion of the characteristics used to summarize each of the operational models, referred to as model characteristics, for whichever characteristics require more explicit discussion than is contained in this chapter; and (5) the summaries of the characteristics of the operational models, referred to as model summary tables.

The characteristics used to describe each operational NSM have been

Figure 2-6. Flow Chart of NSM Selection Procedure


Given: Specification of Required Natural Systems Analysis, as Specified in Step 3 of Steps for Setting Up NSM Analysis
Search Problem Table for Appropriate Models to Address Defined Problems
Are There Models with Desired Attributes?
No
Yes
Go to NSM Summary Tables
Operational Constraints
Specify availability of:
data
personnel
time
computer facilities
money
ADJUST
Yes
Can Additional Resources be Obtained?
No
Are the Available Analytical Resources Sufficient to Implement These Models?
No
Yes
Evaluation Criteria
Compare / Select Model Based on Evaluation Criteria
No
Can Additional Resources be Obtained ?
ADJUST
Yes
Operational Constraints
Specify availability of :
data
personnel
time
computer facilities
money
Specify Model Modification or New Model Development Options and Required Resources
Evaluation Criteria
Are the Available Analytical Resources Sufficient to Modify Existing or Develop New Model?
No
Yes
Complete Model within Operational Constraints
Utilize NSM in REQM Analysis

selected as the most important attributes of NSMs with respect to deciding on the applicability of a model in any given context. Nineteen characteristics have been defined, of which fifteen are applicable to all three NSM categories discussed in this report. Table 2-2 lists and briefly defines the fifteen characteristics which are applicable to all three categories of NSMs. The four which apply to only one specific category are: applicable water body and water body characteristics, applicable to receiving water NSMs; applicable land drainage area, applicable to runoff NSMs; and terrain characteristics, applicable to NSMs of atmospheric systems. Discussions of the last nine of the fifteen--computational status through other comments--are provided in the last part of this section of the chapter. The first six are discussed in each of the next three chapters in relation to specific categories of NSMs, along with any additional comments on the other nine characteristics which are relevant. Detailed summaries of operational NSMs using these characteristics are contained in the appendices to chapters 3, 4, and 5. Although the terminology among the model summary tables is not completely consistent, the terms should be clear.

The NSMs for which summary tables have been prepared are those which--at the time of final compilation in 1978--met the criterion of being operational, and for each of which sufficient documentation was available to enable preparing a summary table. Three comments are relevant with respect to this effort. One, with the finite resources available and the multiplicity of NSM developers and appliers which exists, not all relevant operational NSMs were necessarily "discovered." Two, in some cases, two or even more NSMs are very much alike. It was not considered to

Table 2-2. Identification and Description of Characteristics for Describing NSMs[a]

Characteristic	Summary Description
Time Properties	Description of how temporal variations in flow and/or transport of residuals are represented in a model, both conceptually and computationally. Information includes: (1) time variability: steady state, quasi-nonsteady state, and nonsteady state; and (2) time units of application: input and output values and computational time step.
Space Properties	Identification of capability of model to represent spatial variations of residuals concentrations. Information includes: (1) model dimensionality: one-dimensional, horizontal or vertical plane; or multi-dimensional, longitudinal, latitudinal, and/or vertical plane; (2) spatial aggregation: size and number of segments, layers, and volumes possible; and (3) typical areal units of application.
Physical Properties	Identification of the physical processes considered in a model which account for the transport of residuals. Information includes: (1) the principal hydraulic and meteorologic driving forces, i.e., tidal action, wind currents, and stream currents; and (2) the individual physical processes involved: advection, diffusion, dilution, convection, heat budget-temperature, wind, Coriolis acceleration forces.
Chemical Processes	Description of the chemical transformations/interactions considered in a model which result in changes in concentration over time. Information includes: (1) basic chemical processes: thermo-chemical equilibrium and coupled or noncoupled chemical reactions; and (2) ambient quality indicators represented: conservative substances and nonconservative substances.
Ecological Processes	Identification of basic biological processes that affect interactions between AEQ indicators, constituents, and among the various organisms represented in a model. Included are: (1) biochemical processes, i.e., photosynthesis, respiration-biological decay; and (2) trophic dynamics, i.e., trophic levels, population growth dynamics, mortality, predator-prey interactions.
Mathematical Properties	Description of the theoretical basis for the mathematic representation in, and the solution methodology applied to, a model. Information includes: (1) theoretical aspects: deterministic, stochastic, and combinations; and (2) types of solution methodology: statistical, i.e., regression methods, and other mathematical techniques, i.e., analytically integrated or numerically integrated.
Computational Status	Identification of status of model in relation to manipulation on digital computers. Information includes: (1) whether model is coded or uncoded; (2) computer language used, e.g., FORTRAN; and (3) the various computer/accessory equipment required (hand calculator, analogue computer, digital computer, including needed storage capacity, compilers, magnetic tapes or disks for storage).
Input Data Requirements	Description of the various data required to set up, run, calibrate, and verify a model. Generalized historical data bases and/or site-specific data may be required, depending upon the extent of prior applications.
Ease of Application	Description of expected difficulties in obtaining, modifying, and applying a model. Information includes: (1) the availability of model and supporting documentation from various sources; and (2) identification of anticipated areas of difficulty in model application.
Output and Output Format	Identification of model output with respect to the types of information produced, spatial and temporal distributions possible, and the format in which the output is presented.
Linkages to Other Models	Description of linkages between a model and other types of models used in REQM analysis and the forms of such linkages. Information provided includes linkages to other natural systems models, damage/benefit models, and models of activities and the ways in which the linkages are structured.
Manpower Needs	Identification of types, number, and desired levels of experience of personnel required to apply a model. Requirements for additional model development and/or major internal modification may differ significantly from those for model application. Information includes: (1) position descriptions (engineer, programmer, systems analyst, ecologist, others); (2) need for specialized training or capabilities; and (3) the related experience of interdisciplinary team members.
Costs	Specification of all costs involved in applying a model, from initial acquisition of the model through analysis of model output. Model costs are a combination of: (1) man-hour expense required to complete certain tasks (including data collection); (2) expense of obtaining a model itself and/or available user's manuals/documentation reports; and (3) direct computation costs for the application. Where possible, cost information is provided under the categories of model acquisition, data preparation, actual computation expense, computer accessory costs, and output analysis. Complete cost information is not available for most NSMs.
Model Accuracy and Sensitivity	Description of the overall capability of a model to represent accurately a natural system and its essential processes. Information includes: (1) the representativeness in relation to the "real" system, especially the extent of the description and simplifying assumptions; (2) numerical accuracy--stability and dispersion (in numerically integrated models); and (3) sensitivity to input errors or rate coefficients, both known and estimated values.
Other Comments	Description of miscellaneous facts concerning a model, its history of development and modification, and informative observations as to its utility in REQM analysis. Information includes: (1) model limitations and restrictions; (2) special features and options; and (3) model originators or producer of current derivation (if modification of existing model).

[a] Only those characteristics which are relevant for more than one category of NSMs are included.

be an efficient use of resources to document all NSMs which are essentially the same. Some reference is made to closely related NSMs in the next three chapters. Three, both application and development efforts with respect to NSMs are taking place continually. The set of model summary tables for each analysis category should be considered a base to which additions and deletions should be made as information becomes available.

What is important with respect to the model summary tables is the procedure they represent. Most analysis for REQM involve consideration and manipulation of large amounts of data. Having operational formats for compiling and arranging data can enhance the utility of the data.

Step 5: Model Selection

The fifth step is the selection of the NSM or NSMs to be used in the REQM analysis. This entails applying evaluation criteria to NSMs, after they have been determined to be feasible in terms of available analytical resources, as indicated in the flow diagram of the selection process in figure 2-6. Four evaluation criteria are suggested: (1) accuracy of estimation; (2) capability of estimating AEQ responses to various physical measures for reducing residuals discharges; (3) commonalities which a feasible NSM has with prior natural systems analyses in a region; and (4) contributions that the NSM would make to long-term REQM in a region. It should be emphasized that the level of complexity required to answer the questions in the given context has been specified in step 3, and model costs have been considered in step 4, thereby eliminating these as criteria for evaluation.

Regarding accuracy of estimation, one NSM would be preferred over another if the anticipated range of error--or range of errors--in the first were smaller than the range(s) in the second, provided that the errors fall within acceptable limits. If this condition is satisfied, then the choice between models must be made on other grounds.

The capability of an NSM to estimate AEQ changes in response to the application of various physical measures is an appropriate criterion because NSMs are not equally sensitive to the possible physical measures which might be adopted. For example, a Streeter-Phelps model for BOD and DO, calibrated for a given river under conditions of specified low flow and temperature, might be satisfactory to estimate changes in DO concentration that would result if the physical measures applied only to reducing BOD discharges, under those flow and temperature conditions. However, the model could not estimate AEQ changes that would result from applying physical measures which modified patterns of streamflow or temperature. In most analysis contexts, NSMs which yield estimates of AEQ responses to a broad range of physical measures would be preferred over those with less flexibility.

Commonalities that an NSM may have with prior NSMs used in a region are an important factor. The extent to which an NSM incorporates prior knowledge and experience in a region affects the credibility of model estimates among resident professionals, professionals on whom decision makers rely for technical judgements. Estimates in which resident professionals have little confidence are likely to have little credibility with decision makers, regardless of how accurate the estimates may actually be. Consequently, an NSM which shares processes or variables or both in common with previously accepted analyses will be preferred in many cases over one which hypothesizes relationships and involves variables which have not been tested in the region.

Apart from the utility a given NSM may have for providing information about current REQM decisions, the contributions which it would make to the long-term development of REQM in the region should also be evaluated. As repeatedly stressed, REQM is not a "one shot effort," but rather is a continuing management process. One contribution might be the development of additional technical expertise within a region, another the ability to use an NSM for an additional purpose, e.g., the use of a runoff model to assess flood damage reduction strategies. In a context where spatial and temporal patterns of activities are changing rapidly over time, an NSM which is easily adaptable to new locations of discharges and to a wide range of input environmental conditions would generally be preferred to one which is not.

The foregoing has described proposed criteria for evaluating NSMs for use in REQM analysis. Depending on the context, criteria may be added to, or subtracted from, those identified, and different weights may be assigned to the individual criteria.

Step 6: Develop Work Plan

The sixth step is to develop a work plan to carry out the natural systems analysis. Various formal procedures for preparing such plans are available. What is critical is that the work plan must mesh with the work plans for other segments of the REQM analysis; certain analytical tasks must be accomplished before others can be initiated. The NSMs must be ready before any analysis of the effects of combinations of physical measures is possible. Table 2-3 summarizes the steps in setting up the analysis of natural systems.

Characteristics for Describing NSMs

The comments on the following characteristics are relevant for all NSM categories. Specific comments on these characteristics for individual categories of NSMs are contained in the following three chapters, where relevant.

Computational Status

This characteristic indicates whether the theoretical model framework, e.g., equation sets, has been translated into an operational model. Most operational models are coded, i.e., translated into a computer language or appropriate computational format. Uncoded models are generally not operational in relation to REQM analysis because they are at a preliminary development stage, where mathematical descriptions have not yet been placed in a functional computational format.

Other important features of a model's computational status include the type of computer language used and the computational equipment needed to execute the model. FORTRAN IV is the predominant computer language currently used for receiving water models, although other languages have been used, e.g., PL-1 has been utilized in some aquatic systems modeling. The make and type of computer available for a given REQM analysis may be an important operational constraint. Information relating to storage and operating capacity of available computers is often necessary to determine the feasibility of implementing a particular model.

Table 2-3. Summary of Sequence of Steps for Setting up the Natural Systems Analysis

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Given: The "questions" to be addressed by the study have been identified and translated into specific information requirements to be generated on AEQ, distributions of AEQ, and REQM costs. The residuals of concern, relevant time periods, and boundaries of the study area for which information is required have been specified.

Step 1: Make a preliminary identification of the environmental media and relevant characteristics thereof that are affected by the residuals of concern, e.g., by considering known transport pathways, impacts of residuals on relevant species, accumulation and/or degradation of residuals in environmental media, and a determination of the categories of natural systems analyses--residuals generation/discharge, surface receiving water, terrestrial flow routing, subsurface flow, terrestrial ecologic, and atmospheric ambient quality--that are necessary to undertake in relation to the questions to be answered.

Step 2: Based on the foregoing and on available data on environmental conditions variables, residuals discharge variables, and AEQ variables, make a preliminary analysis in order to determine: (1) if the right questions have been asked; (2) if the important residuals have been identified; (3) the relative importance of various point and aerial sources of residuals; (4) the potential importance of intermedia and interregional transfers; and (5) any additional characteristics of the problem which will help to determine the NSM(s) to use.

Step 3: Based on the results of step 2, specify the level of complexity desired for the natural systems analysis in terms of: (1) time intervals of analysis, i.e., hourly, daily, monthly, seasonal, mean annual; (2) spatial aggregations, i.e., number of grid areas, stream reaches, lake layers; (3) constituent/species aggregations to be considered, i.e., forms of nitrogen, number of fish species; and (4) specific physical, chemical, and biological processes to be incorporated.

Step 4: Determine the feasibility of carrying out the natural systems analysis specified in step 3, in relation to the available analytical resources. In order to determine feasibility, see relevant chapters on natural systems categories for choosing among presently existing operational models utilizing a model selection procedure, a model population table, a model problem table, model characteristic, and model summaries. Note that iteration may be necessary in order to make the choice of NSM(s) consistent with the available analytical resources.

Step 5: Select the NSM or NSMs to be used based on the relevant evaluation criteria.

Step 6: Develop a work plan for the natural systems analysis which is compatible with other segments of the REQM analysis.

Input Data Requirements

This characteristic identifies the types and amounts of data that are required to execute a model properly. Depending upon the number of interactions that are explicitly considered within a model and the solution technique(s) employed, data requirements will vary greatly among operational models.

Data requirements are grouped into two major categories: (1) data required for model setup and calibration; and (2) data required for model verification. Most of the data necessary to implement a model are required for model setup and calibration. Setup and calibration usually require the construction of a data base which describes the physical, physical and chemical, or physical, chemical, and ecological relationships of the natural system to which a model is to be applied. Initial setup data required also include the available historical record for spatial and temporal patterns of residuals discharges, AEQ indicators, and environmental conditions variables. Additional data usually are also needed to generate internal model coefficients, such as decay/degradation rates in receiving water models.

For model verification, a completely different data set is required. Although the data required for model verification can be much more limited in scope than the data required for setup and calibration, the data must be collected at the same locations which are used to present the model output. This usually requires a monitoring program specifically aimed at providing the requisite verification data.

Ease of Application

This characteristic provides information on how and where to obtain a given NSM and the documentation needed to facilitate application. The major elements of this model characteristic are: (1) the availability of the model and its supporting information, that is, user's manuals, reports of previous model application, documentation reports; (2) the extent and sufficiency of that information; and (3) the expected difficulties in applying the model.

In fact, most models cannot be "taken off the shelf" and applied directly without some modification. User's manuals, detailed documentation reports, and model development study reports are therefore necessary to convey the model's theoretical and conceptual basis, describe its basic assumptions and limitations, and present instructions for modifying or updating program files, subroutines, data decks, and other operational features. Without such aids, the process of "debugging" and applying an NSM can be lengthy, expensive, and sometimes unproductive.

NSMs have historically been developed by governmental agencies, academic institutions, and private consulting firms. Obtaining an operational model from a public governmental agency is perhaps the easiest solution, because many agencies publish reports on models developed in-house or on a contractual basis. Governmental publications often may be obtained free from agency contacts or at nominal cost from the National Technical Information Service (NTIS) if out-of-date. Unpublished contract reports and computer printouts of program files, data, and subroutines may be more difficult to obtain unless the exact reference to or location of the material sought is known. Modelers at academic institutions often publish articles at various stages of the model development process, but rarely are complete documentation reports available for even the most practical research models. Consulting firms may have proprietary models developed with private funds; however, many of their model development projects have historically been funded by governmental agencies and are considered part of the public domain.

The extent and sufficiency of model documentation is quite variable, but the availability of useful model information, such as detailed user's manuals, will directly aid the user in setting up and operating a model and will minimize the time and manpower requirements needed to implement a given model. Good documentation consists of: (1) discussion of model theory, i.e., conceptual basis, equation sets, and solution methodology; (2) fully identified assumptions and limitations; (3) complete program listings; (4) efficient subroutines, data deck design, and instructions for modification; and (5) identification of potentially troublesome coefficients, functions, or variables. Often all this information is not conveniently provided in a single source, so pertinent documents must be obtained from continuing research and development activities and different model applications prior to undertaking the specific model application.

Output and Output Format

The types of output that can be produced by a model comprise an important consideration in selecting a model for use in REQM analysis. The specific output information, in terms of residuals considered and spatial and temporal patterns, e.g., of concentrations, varies from model to model.

The format in which model output is produced can be very important to the user, particularly for simplifying data interpretation and for presenting results. The types of output formats that can be produced by a given model are indicated under this characteristic. For example, a printout with lengthy tabular listings may be complete in terms of describing residuals or AEQ levels at all relevant points. However, the lack of summaries of such output data often increases manpower requirements for analyzing the output and presenting results.

Linkages to Other Models

No NSM is applied in a vacuum. Therefore, it is important to know how a given NSM can be integrated with other segments of the REQM analysis. As indicated in chapter 1, one of the inputs to NSMs is comprised of the outputs, i.e., residuals discharges, of the analyses of residuals generating activities. Similarly, in order to estimate damages and benefits, the outputs of the NSMs are inputs to damage and benefit models. In addition to these backward and forward linkages, often there are "sideward" linkages, from one NSM to another, within the same category of NSMs or from one category to another.

Manpower Needs

The types and amounts of manpower required to implement an NSM are a function of five factors: (1) model operational status and availability of associated documentation; (2) the state of needed data, i.e., availability, quantity, quality, additional analysis needed; (3) the complexity of mathematical formulations and the solution techniques under consideration; (4) the space and time units used; and (5) the output options available, and required in a given context. For comparing manpower needs among different NSMs, these needs are best described in terms of type and capability of personnel, e.g., position descriptions, training, and experience.

The types of technical expertise required are contingent upon the specified AEQ problems and the inherent characteristics of the NSM being evaluated. For example, application of a simple steady state receiving water model might require a programmer with only rudimentary training in FORTRAN programming, whereas a finite element model of a complex estuarine system would necessitate close cooperation between an experienced programmer and a competent hydraulic engineer or ecologist.

The ultimate size of the team required for analyzing natural systems also depends upon the NSM(s) to be used. Personnel with specialized training and experience in both the engineering and scientific disciplines related to the environmental media involved are especially important at certain stages of the NSM analysis, e.g., initial model setup, "debugging," calibration, and verification.

Conceptually, the same personnel capabilities are required whether in-house personnel or consultants are used. However, tradeoffs may be possible, between staff personnel with less experience--so that a longer time would be required for analyzing the relevant natural systems--and more experienced consultants who could do the analyses more quickly but at higher unit costs. Total costs for the NSM segment might be essentially the same. In that case, the time to accomplish the analysis and the longer term benefits from increasing the capability of the staff personnel might well become the deciding factors.

Model Costs

The cost of utilizing a particular NSM is dependent to some extent upon features discussed under other model characteristics. The total cost of a model application can be separated into model setup costs and model utilization costs.[9] These categories involve the steps in the model implementation process: (1) model acquisition; (2) familiarization, setup, and data preparation; (3) calibration and debugging; (4) actual computation; (5) verification; and (6) output analysis.

Describing and estimating costs for applying an NSM is difficult and perplexing, because of the lack of cost information in the literature. For example, simple cost indices such as dollars per run--often expressed as a range--are satisfactory when comparing the amount of computer time needed to apply a similar set of input conditions for similar models. However, as a basis for explaining differences in costs, such as those resulting from model complexity, extent of discretization (disaggregation), or even inefficient computation routines, such simple indices are inadequate. Because of the paucity of information about costs in the model summary tables, a simple cost formula is presented to assist in estimating the cost of implementing a given NSM in any given context.

To calculate the total cost of a given model application--not just a single simulation run--the individual costs of a series of model-related costs must be estimated. These individual cost components are shown in the following simple formula:

Modeling Application Cost = model acquisition costs + personnel costs + computing equipment charges

where, model acquisition costs = leasing arrangements, if relevant; documentation, printout, and report charges; reproduction costs, if documentation reports are unavailable; mailing or shipping costs; consultation fees, if relevant;

personnel costs = number of staff persons needed; position descriptions and applicable salary rates; time expended per task (person-days); model familiarization; data preparation; model setup, debugging, and data revision; calibration, verification; output analysis; and

computing equipment charges = computer rental or lease arrangements, where cost depends on factors such as equipment capacity; computer connect time and model execution time which are a function of length of equation sets, number of time steps, and extent of discretization; software and accessory costs, such as keypunching, terminal rental, compiler lease; disk purchase and storage fees; printout and graphics' expenses including delivery charges and customer support services.

Three points concerning model costs merit emphasis. One, a partially operational model will cost more in manpower and computer charges than a fully operational model, because of the number of additional computer runs that a modeler must conduct in order to upgrade such a model into an operational model. Two, to obtain information on model costs, in many cases model developers, model users, or both will have to be contacted directly. Three, of the three components in the above equation, personnel costs will dominate in almost all situations.

Model Accuracy and Sensitivity

The sensitivity of an NSM to various variables--both endogenous and exogenous--is an important characteristic. Operationally, sensitivity analysis with respect to NSMs is defined as the investigation of changes in values of AEQ indicators which result from changes in values of independent variables and in the posited relationship among model variables. An independent variable has more or less relative importance depending on the impact it has on the dependent variable. Consequently, the extent to which the more important dependent variables can be accurately estimated has significant impact on the accuracy of the NSM. The sensitivities of certain variables in various models are reported in the model summary tables where such information was available.

In addition to the obvious importance of the quality of input data, the accuracy with which an NSM estimates AEQ depends on: (1) the extent to which the model represents the actual natural system; and (2) the accuracy of the solution technique employed. The accuracy of the solution technique employed is relevant for models based on conservation of mass and energy which are solved using numerical integration methods.

The extent to which an NSM represents the actual system to which it is applied depends on the theoretical formulation of the model, i.e., the variables and the relationships among variables represented. Sometimes this type of information is buried in complex mathematical formulations and is obvious only to experienced model users. Where possible, comments as to deficiencies in representation of actual systems are reported in the model summary tables.

The accuracy of a numerical integration method is affected by two factors, stability and convergence. Stability refers to the ability of a numerical integration method to iterate to a solution, given the time step and spatial discretization required in a given context. Convergence refers to the cumulative mathematical errors resulting from numerical approximations, which errors are an inherent property of numerical integration methods. The errors vary from model to model. To the extent possible, information on these two factors is reported.

Other Comments

This is a category provided to enable recording of information which does not fit readily under one of the other characteristics. Examples of information appearing under this heading include: (1) model restrictions and limitations; (2) special features of models, e.g., some receiving water models have flow augmentation options to evaluate various flow patterns; and (3) information about model developers. If a model is a modified version of another operational model, this fact would also be indicated here.

Summary Comments on Characteristics

It should be emphasized that the characteristics discussed above are relevant not just to the models contained in the appendices to the next three chapters, but are relevant for all NSMs. As such, the characteristics and the framework within which they are presented serve as a general basis which can be used to summarize NSMs. This basis is useful in and of itself because it provides individuals and organizations with a consistent means to summarize NSMs for the purpose of comparison.

SOME PROBLEMS IN ANALYZING NATURAL SYSTEMS

Regardless of the category or type of NSM, a number of common problems exist with respect to adoption, operation, and utility of models. Raising these underscores the difficulty of selecting, modifying, or developing appropriate NSMs for any given REQM analysis. This section describes briefly five problems. The order of discussion does not imply order of importance.

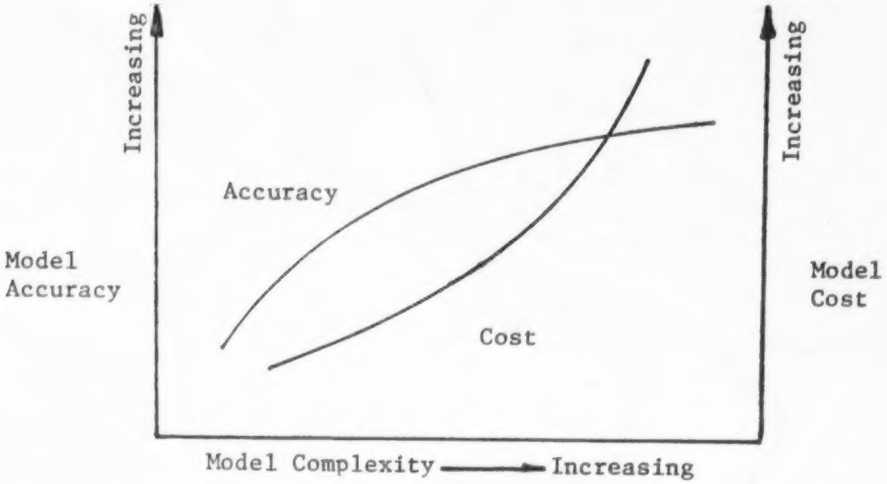
Complexity of Natural Systems Models

A critical problem in any REQM analysis is determining how complex an NSM to use in the analysis. Four facets of model complexity can be identified. These are: (1) the relationship between model complexity and model accuracy, where accuracy is determined by the closeness to which the observed AEQ is estimated, using one or more indicators of AEQ; (2) the relationship between model complexity and model cost; (3) the relationship between model complexity and the amount of information generated--both level of detail and scope--with respect to the question(s) being addressed; and (4) the relationship between model complexity and the degree to which observed data are available for model calibration and verification.

Model complexity is defined to be a function of: (1) the number of variables explicitly included in the model structure, and (2) the accuracy of the estimates of the values relating to each of those variables. Presumably the accuracy with which an NSM predicts the value or values of one or more indicators of AEQ increases as model complexity increases. But with increasing complexity, the rate of increase in accuracy diminishes and the cost of modeling increases, as depicted in figure 2-7. In fact, accuracy may actually decrease if the model becomes so complex that it is unstable or cannot be understood.

Increasing model complexity often increases the amount of information produced. For example, a Streeter-Phelps model yields only estimates of dissolved oxygen (DO) and five day biochemical oxygen demand (BOD_5) concentrations, whereas an aquatic ecosystem model might yield not only DO and BOD_5 concentrations, but also algal concentration, biomass of fish, and turbidity.

Figure 2-7. Relationships Among Model Complexity, Model Accuracy, and Model Cost



The complexity of an NSM to be used in a given case depends primarily on the question(s) being addressed. If the issue were the impact on a particular species of fish, then a simple BOD_5-DO model is likely to be insufficient. On the other hand, if BOD_5 and DO concentration were adequate measures of water quality in relation to recreational use, then the simple BOD_5-DO model would be sufficient. If the objective were to obtain an approximate estimate of mean annual concentration of SO_2 in a metropolitan area, a simple box model might be sufficient, rather than a complex conservation of mass model which would require the delineation of specific residuals discharge locations and specific locations for which ambient concentrations would be estimated.

The complexity of a natural systems model to be used in a given case depends also on the accuracy of the model relative to the accuracy of the residuals discharge data generated by the analysis of residuals generating activities. There is no point in having a very complex NSM if the accuracy of the residuals inputs generated by the analysis of activities is low.

Finally, if empirical data to calibrate and verify an NSM are limited, there is little point in developing a complex model. In such cases there is no way to determine whether a complex model is a better predictor of impacts on AEQ than a simple model.

Calibration and Verification[10]

Calibration and verification are sequential but separate steps that are required before an NSM can be used to estimate the impacts on AEQ of: (1) residuals discharges; (2) applying physical measures for reducing residuals discharges; and (3) applying measures for directly modifying assimilative capacity. Calibration is the process of using a set of observed data to adjust an NSM--structure, internal coefficients, or both--so that the values of the AEQ indicators estimated by the model are within acceptable limits to observed values of AEQ, for the given set of values of the independent variables. If the differences between estimated and observed AEQ are greater than the limit(s) established by the individuals calibrating the model, the NSM is considered unacceptable and must be investigated for possible causes of error. Three primary sources of error are: (1) inaccurate input data; (2) inaccurate internal coefficients; and (3) inadequate model structure (specification).

After adjustments are made, the model is run again, and the new estimates of AEQ are compared to the observed values. The process is repeated until: (1) estimated AEQ falls within the specified limits of accuracy; or (2) all known errors have been eliminated and the estimated values are still not acceptable. In the latter case the NSM would be abandoned.

It is important to emphasize that the temptation often exists to make "ad hoc" or "trial and error" adjustments to an NSM during the calibration process, adjustments which have no scientific justification. Such a procedure should be avoided.

Verification is the process of using a set of observed data different from the set used in calibration, to compare estimated values of AEQ with observed values of AEQ. If the differences between estimated and observed AEQ fall within specified limits, then the model is said to be "verified" and is ready for use. If differences between estimated and observed AEQ are greater than the limits specified, the model should not yet be applied. The possible sources of discrepancies must be identified. In some cases the cause will be errors in the new data; in others the model may have to be recalibrated, perhaps modified, and then reverified; in still others, the model may have to be abandoned.

Two common and major problems affecting calibration and verification of NSMs warrant discussion. The first is the lack of adequate data, particularly independent sets of data. Seldom are sufficient data available to satisfy the needs of both calibration and verification. Consequently, data required for calibration and verification must be explicitly considered in the decision to adopt or develop a given NSM. No NSMs which have not been calibrated and verified should be used in a final REQM analysis.

The second is the specification of acceptable limits of accuracy for an NSM. In general, most presently operational NSMs are relatively inaccurate in relation to conventional notions of accuracy. For example, in applications of Gaussian air quality models to metropolitan regions for estimating seasonal averages of air quality indicators, acceptable accuracy is considered to have been achieved when estimated values are within a factor of one or two of the observed values. In an NSM which estimates values of more than one indicator, different accuracy limits can be specified for different indicators. Limits of accuracy should be set in relation to: (1) the accuracies of other segments of the REQM analysis; (2) the question(s) being asked; (3) the accuracies of the field measuring equipment and of laboratory analyses; and (4) the levels of accuracy attainable with the NSMs.

Background Concentrations of Residuals

Background concentrations refer to ambient concentrations of residuals which result from sources for which no explicit estimates of discharges from individual sources are made or for which no explicit physical measures to reduce discharges are considered in the REQM analysis. These sources include: (1) natural sources within the region; (2) activities of man within the region which are so small that the discharge from each individual activity is insignificant but when added to all other similar discharges may become significant; and (3) sources outside the region, i.e., cross-boundary transfers of residuals. The third can be comprised of any one or a combination of single major sources, natural sources, and many small scale sources. Operationally, in any given REQM analysis, all of the above sources may be incorporated in the background concentrations, and no measures to reduce discharges from these sources would be included.

Because background concentrations represent the portion of AEQ which will be unaffected by residuals discharge reduction measures applied in a given region, it is important that they be accurately estimated.

Operationally, background concentrations represent the upper bound of AEQ improvement that is attainable by adoption of physical measures within the region, because if residuals discharges from all of man's activities in a region were reduced to zero, AEQ would reflect only background concentrations. The intra regional natural sources and the extraregional sources may be large enough so that AEQ standards within the region cannot always be achieved even with zero discharge from each of the activities within the region.

The foregoing are important considerations in setting up the REQM analysis and in setting up the natural systems analysis. If a significant portion of AEQ is contributed by sources external to the region, the REQM analysis--and the NSMs used therein--will likely have to include at least the major sources beyond the regional boundaries originally defined. For NSMs based on the mass balance principle, it is particularly important to specify background concentrations and related boundary conditions accurately, to ensure the integrity of mass balance equations.

Linkage Between NSMs and the Analysis of Activities

The linkage between NSMs and the analysis of activities is another critical aspect of the analysis of natural systems. The analysis of activities provides the requisite residuals discharge data as inputs into NSMs. Consequently, the accuracy of the outputs of any given NSM depends on the accuracy of the residuals discharge data generated in the analysis of activities. A problem arises when the NSM to be used requires residuals discharge data which are more accurate than the data which can be provided by the analyses of activities. This is more frequently a problem than is commonly recognized. For example, an air quality model used to analyze an episodic condition, i.e., three or four days of extremely poor air quality, will typically employ an averaging time of one hour or less. However, very rarely is it possible to estimate hourly variations in residuals discharges for: (1) all--or even the most important--activities in a region, including natural sources; and (2) sources outside of the region. In such cases residuals discharges are usually assumed to be constant over some time period and an average hourly discharge rate is estimated and used as the input into the NSM. The impact on the accuracy of the output of the NSM will vary depending on the NSM, the types of activities in the region, the importance of the background sources, the importance of sources outside the region, the nature of the problem, and meteorological conditions.

Two exceptions should be mentioned. One is the case of photochemical "smog." The principal residuals of concern in this problem--oxides of nitrogen and hydrocarbons--are discharged primarily by motor vehicles. Variations in residuals discharges from motor vehicles are usually estimated from traffic count data, i.e., observations of the time pattern of numbers and types of vehicles passing given points. Hence, variations in residuals discharges can be estimated to match averaging times of one hour or less used in photochemical reactive air quality models. (Such models are described in chapter 5.) A second exception is when a runoff model--used to estimate residuals discharges into a surface receiving water model--has the same averaging time as the surface receiving water model. An example would be a runoff model which yields estimates of residuals discharges into a surface receiving water body on an hourly basis, for given meteorological conditions, and the receiving water model yields estimates of changes in AEQ indicators on an hourly basis.

The problem of relative accuracy becomes especially acute when NSMs are used to analyze the impacts of future levels and spatial patterns of activities on AEQ. Estimates of future spatial patterns of activities are usually based on some form of an economic-demographic projection/allocation model. Given the inherent inaccuracies of such models, especially as the time horizon lengthens, the information produced by these models in terms of aggregations of activities and the spatial distribution of the activities rarely, if ever, coincides with the aggregations required for making estimates of residuals discharges for input into NSMs. For example, most economic-demographic projection/allocation models disaggregate activities according to two or, at best, three digit Standard Industrial Classification (SIC) categories, and at best spatially disaggregate data to the county level. Numerous assumptions regarding the characteristics of activities within SIC categories and locations of those activities within counties are required. Thus, it is not at all clear what level of complexity of NSMs is logical when analyzing conditions 15 or 20 or 25 years in the future.

Interpreting Results of Applying NSMs

As indicated previously, the accuracy of the outputs of most NSMs is at best only a factor of 2. This is partly attributable to the accuracy of input data. The previous section discussed the accuracy of input data in relation to estimates of residuals discharges. But regardless of the accuracy of the input data, NSMs are only abstractions of reality. Herein lies the difficulty of interpreting the results of applying them.

First, in the real world the chemical, biochemical, physical, physicochemical, and ecological processes at work are stochastic phenomena. But practically all operational NSMs currently available consider these processes and related relationships to be nonstochastic. Second, most relationships among variables in natural systems are nonlinear, but for computational convenience are formulated as linear relationships in many NSMs. Nonlinearities result in significant computational problems in REQM analyses of other than the most simple regions.[11] Third, there may well be more relevant variables in "real world" natural systems than can be incorporated in an NSM. Finally, the calibration and verification of an NSM is always done for some range of conditions for which data are available. The set of conditions estimated for some point in time in the future may lie sufficiently far outside that range that the NSM may no longer be valid.[12]

Given these factors, one way to enhance the interpretation of results in applying NSMs is to investigate the sensitivity of model outputs to changes in values of input variables and in the structure of the model itself. This is commonly referred to as sensitivity analysis. To repeat, sensitivity analysis of NSMs is operationally defined as the investigation of changes in values of AEQ indicators which result from changes in values of independent variables and in the posited relationship among the model variables. The relative importance of an independent variable depends on the impact it has on the dependent variable. The variable resulting in the largest change in the dependent variable for a unit change in its own value is the most important.

Sensitivity analysis in and of itself can be a difficult analytical task, but it is nevertheless an important tool for evaluating results.

At the very least it is important to identify which are the most important variables affecting estimates of AEQ, because low accuracy in these variables will yield low accuracy in the estimates of AEQ. Sensitivity analysis can indicate where more data collection, respecification of relationships in the NSM, or both, can improve accuracy and hence overall results.

To the extent possible, information regarding model sensitivity is provided for each of the operational NSMs summarized in the appendices of the following three chapters.

Concluding Comments

The foregoing discussion makes it clear that a staff of competent professionals is required in order to apply, modify, and develop NSMs for use in REQM analysis. Regardless of the level of complexity of an NSM, skilled individuals will always be required to exercise the judgment necessary to apply the model and to interpret the results produced. Even for the operational models currently available, only some are truly adequately documented. It cannot be overemphasized that models are just tools; they are not substitutes for a professional's skill, experience, and understanding. It follows that the decision to adopt, modify, or develop an NSM will inevitably require a sizeable initial commitment. However, once set up, calibrated, and verified, an NSM is a necessary and powerful tool for assessing the impacts on AEQ of alternative REQM strategies.

NOTES

[1] Noise transmission models can be considered a subcategory of atmospheric models. Noise transmission models are not discussed in this report.

[2] For a mid-1980 status report on long-range transport models see Michael (1980).

[3] Varied terminology is used in the literature to identify these approaches and variants of them. An approach frequently referred to in the literature as "empirical," based on observation and experiment, is herein considered a variant of the statistical approach. However, the application of all approaches is empirical in the sense that data from observations of "real" systems are used.

[4] For a cogent discussion of stochastic streamflow inputs for analysis of water resources systems, see Thomas and Fiering (1962).

[5] Particularly for preliminary analyses, the assumption is sometimes made that the natural system, for example, an airshed or a small lake, is a "mixing bowl." This means that all discharges of a given residual, wherever located within the natural system, are assumed to be uniformly mixed within the specified volume, thereby yielding an homogenous concentration throughout the volume.

[6] Regardless of the number of dimensions included in the NSM, the natural system is divided into volumes or spaces, as shown in figure 2-2.

[7] Many references describing regression analysis and other statistical methods in detail are available. For example, see Kmenta (1971) and Miller and Freund (1965).

[8] Included are the data required for calibration and verification of any NSM to be used, an important and often overlooked requirement.

[9] Tradeoffs between model setup costs and model utilization costs may be possible. That is, a model which requires more resources to set up may have lower computational costs, and the reverse.

[10] The term "validation" has been, and is, used in connection with calibration and verification. In some cases validation has been used to refer only to verification; in other cases it has been used to refer to calibration plus verification. To avoid confusion, the term is not used herein.

[11] For an excellent discussion of this point, see Spofford, Russell, and Kelly (1976) chapter X.

[12] For example, many air quality models are verified only in the sense that they predict spatial/temporal patterns of ambient air quality in relation to the existing pattern of discharges. This does not mean that they are verified for conditions involving changed patterns of discharges. This limitation is particularly important for ozone models.

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Appendix A

LISTING OF MODELS AND REFERENCES PERTAINING TO PRELIMINARY ANALYSIS

This appendix provides information regarding natural systems models which can be used for preliminary analysis of residuals generation and discharge from land surfaces, receiving water systems, and atmospheric systems. NSMs which are suitable for this purpose and are summarized in the next three chapters are included in the listing below along with some selected references.

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Suitable Models Summarized in Appendix A to Chapter 3

- Environmental Pollution Assessment - Erosion, Sedimentation and Rural Runoff Model, National Environmental Research Center, Environmental Protection Agency, Athens, Ga. (Requires digital computer.)
- Hydroscience Simplified Model, Hydroscience, Inc., Westwood, New Jersey. (Requires electronic calculator.)
- Midwest Reserach Institute Loading Functions, Midwest Research Institute, Kansas City, Mo. (Requires electronic calculator.)
- Simplified Storm Water Management Model (Simplified SWMM), Metcalf and Eddy, Inc., Palo Alto, Calif. (Requires digital computer.)

- Storm Water Management Model, Level I (SWMM-Level I), Department of Environmental Engineering, University of Florida, Gainesville, Fla. (Requires electronic calculator.)

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Suitable Models Summarized in Appendix A to Chapter 4

- Dissolved Oxygen Sag Model (DOSAG I), Texas Water Development Board, Austin, Texas. (Requires digital computer.)
- Revised Oxygen Sag Model (DOSAG II), Water Resources Engineers, Austin, Texas. (Requires digital computer.)
- Simplified Estuary Model (SEM), Hydroscience, Inc., Westwood, New Jersey. (Requires electronic calculator.)
- Simplified Stream Model (SSM), Hydroscience, Inc., Westwood, New Jersey. (Requires electronic calculator.)

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Suitable Models Summarized in Appendix A to Chapter 5

- Croke-Roberts, Energy and Environment Systems Division, Argonne National Laboratory, Argonne, Ill. (Requires electronic calculator.)
- Gifford and Hanna Volumetric Model, Atmospheric Diffusion Laboratory, Oak Ridge National Laboratory, Oak Ridge, Tenn. (Requires electronic calculator.)
- Oak Ridge Fog and Drift Model (ORFAD), Oak Ridge National Laboratory, Oak Ridge, Tenn. (Requires digital computer.)
- PTMAX Model, PTDIS Model, PTMTP Model, and HIWAY Model, Meteorology Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, N. C. (All require digital computer.)
- Rollback Appendix J, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, N.C. (Requires no computational aids.)

Appendix B

ANALYZING TERRESTRIAL ECOSYSTEMS

Melvin O. Hinson, Jr.

TERRESTRIAL ECOSYSTEMS IN REQM ANALYSIS

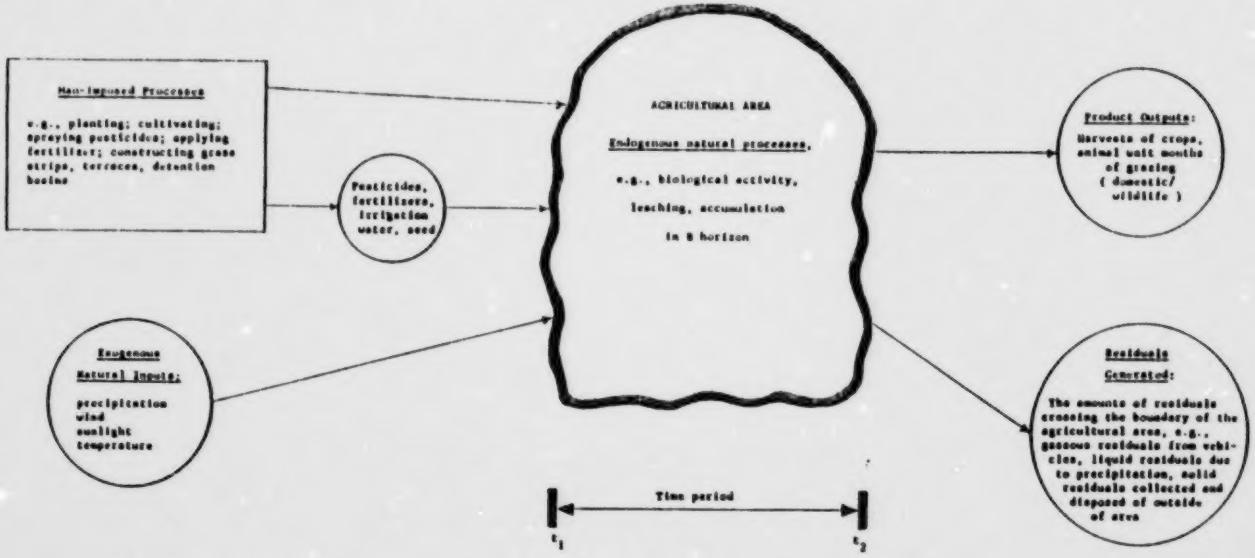
The terrestrial ecosystem, as defined for REQM analysis, is comprised of the plant and animal communities residing on the land surface and the complete set of physical, chemical, and biological processes that interact with and comprise the interactions among those communities. Terrestrial ecosystems are closely linked to ecosystems in surface waters, to groundwater systems, and to atmospheric systems through common sets of interacting physical, chemical, and biological processes, e.g., nutrient cycles, hydrologic cycle, heat budgets.

A variety of different terrestrial ecosystems covers the land surface, each with a distinctly different set of characteristics. Prairies and grasslands, coniferous forests, deciduous forests, semi-arid brushlands, marshes, and swamps are examples of major types of terrestrial ecosystems and illustrate the diversity of undisturbed North American ecosystems. Whereas the original spatial patterns of terrestrial ecosystems on the land surface of the North American continent were dictated by long-term climatic conditions and natural patterns of vegetative succession, the present pattern of terrestrial ecosystems, in any given area, is most often the result of cumulative alterations to the original pattern because of man's activities over time. Agricultural operations, commercial logging, land clearing for urban development, are examples of activities which man has superimposed over existing ecosystems with consequent alterations in those ecosystems.

The role of modeling terrestrial ecosystems in REQM analysis is illustrated by the representation of an agricultural area in figure 2-8. Acting upon the area are exogenous natural inputs, man's inputs, man-imposed processes, and the natural processes endogenous to the area. Outputs from the agricultural area are yields of desired products and residuals. All of these interact to result in alterations--or in some rare cases, maintenance--of the terrestrial ecosystem. The objective of explicit analysis of terrestrial ecosystems is to provide better estimates of both product yields and of residuals generation. For example, the interaction noted above may affect infiltration capacity of the soil, which in turn affects runoff and residuals generation.

Modeling of terrestrial ecosystems could, conceptually, be useful in a variety of REOM analysis contexts, for example: prediction of whether native vegetation can be reestablished on strip-mined land in semi-arid areas; estimation of inputs required over time to maintain intentionally altered ecosystems, as illustrated in figure 2-9, and the associated residuals generated over time; estimation of the changes in an alpine ecosystem under recreational use of specified intensity and the resulting residuals generated; and estimation of the changes in a high desert ecosystem as a result of the impacts of off-road vehicles and the resulting changes in residuals generation, such as wind-generated airborne particulates. In all cases the question is: what degree of detail in the model of the terrestrial ecosystem is necessary for a given REQM analysis?

Figure 2-8. Illustration of One Context of Analyzing Terrestrial Ecosystems: An Agricultural Activity


Man-Imposed Processes
e.g., planting; cultivating; spraying pesticides; applying fertilizer; constructing grass strips, terraces, detention basins
Pesticides, fertilizers, irrigation water, seed
Exogenous Natural Inputs:
precipitation
wind
sunlight
temperature
AGRICULTURAL AREA
Endogenous natural processes,
e.g., biological activity,
leaching, accumulation
in B horizon
Product Outputs:
Harvests of crops, animal unit months of grazing (domestic/ wildlife)
Residuals Generated:
The amounts of residuals crossing the boundary of the agricultural area, e.g., gaseous residuals from vehicles, liquid residuals due to precipitation, solid residuals collected and disposed of outside of area
Time period
t_1
t_2

SOS = state of the system.

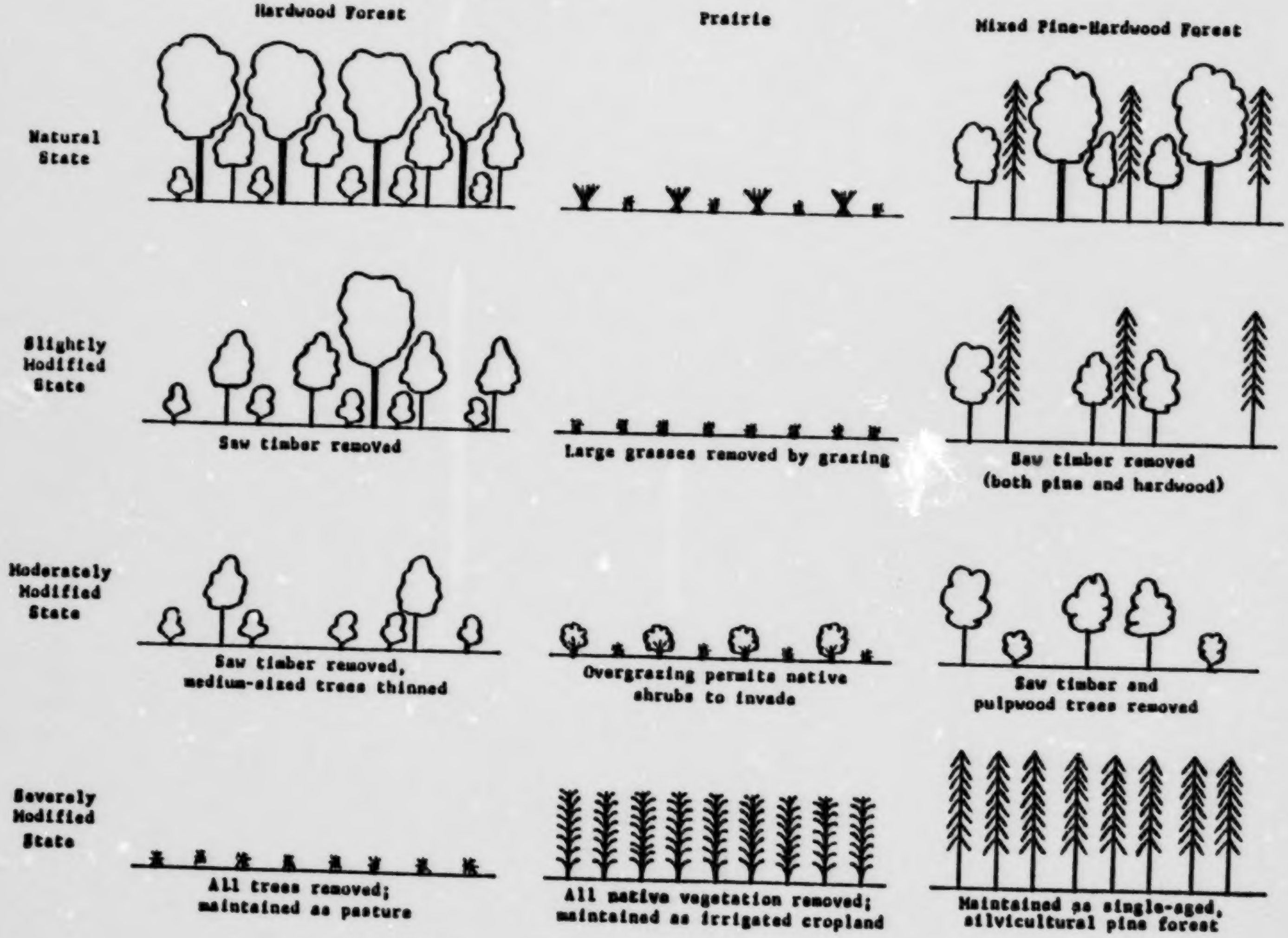
SOS is measured by, for example, amount of organic matter in A horizon, chemical content in A and B horizons, soil texture, drainage characteristics.

Inputs act on and outputs are produced from the agricultural area over time period, $t_2 - t_1$

SOS at t_2 = f(SOS at t_1, exogenous natural inputs, man-imposed processes and inputs, endogenous natural processes, product ouputs, and residuals generated).

Note: Rectangle represents a set of unit processes and operations applied to the agricultural area
Circles represent inputs and outputs.

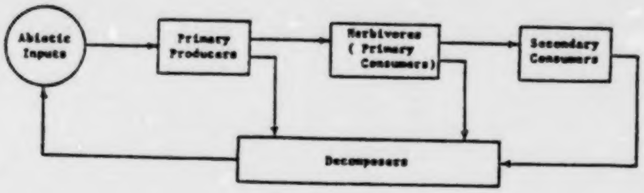
Figure 2-9. Illustrative Examples of Three Natural Ecosystems and the Modified Systems Resulting from Various Intended Alterations


Hardwood Forest
Prairie
Mixed Pine-Hardwood Forest
Natural State
Slightly Modified State
Saw timber removed
Large grasses removed by grazing
Saw timber removed (both pine and hardwood)
Moderately Modified State
Saw timber removed, medium-sized trees thinned
Overgrazing permits native shrubs to invade
Saw timber and pulpwood trees removed
Severely Modified State
All trees removed; maintained as pasture
All native vegetation removed; maintained as irrigated cropland
Maintained as single-aged, silvicultural pine forest

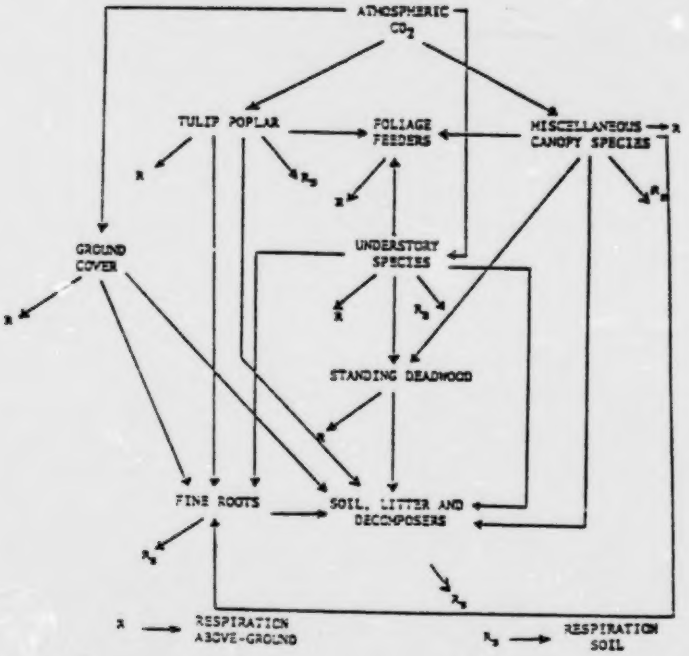
Figures 2-10a and 2-10b illustrate two levels of complexity in modeling terrestrial ecosystems. Figure 2-10a shows the minimal components (represented by boxes) and pathways (represented by arrows) necessary to represent a complete terrestrial ecosystem. Figure 2-10b illustrates a more disaggregated representation. Each pathway between components involves a specific ecologic process or aggregated set of processes whose rate may vary with ambient conditions, such as temperature, humidity, soil moisture, and light intensity. For example, the pathway in figure 2-10a between herbivores and carnivores (secondary consumers) implies the total consumption of the herbivores as food by all other animals. In a more detailed representation, this pathway is actually numerous pathways, each describing consumption of one species of herbivore by one species of carnivore. The actual number of components and transfer paths in any given ecological model will vary depending on the type of conveyance and the REQM context.

A model of a complete terrestrial ecosystem must be comprised of three groups of organisms: (1) primary producers, i.e., green plants that utilize sunlight, carbon dioxide, and soil nutrients to produce their own organic matter via photosynthesis; (2) secondary producers, i.e., animals that consume organic matter of plant or animal origin; and (3) decomposers, i.e., microbial organisms that consume waste organic matter and release the original nutrients as respiration byproducts.[1] Omission of one or more of these groups means that a subset of natural processes is not being considered. In such cases, analyses are limited to individual organisms or to interactions between two or more different species of organisms, termed the population level, rather than the ecosystem level, i.e., considering interactions among all species. The extent to which these three groupings are disaggregated from homogenous groups into individual species with

Figure 2-10. Conceptual Representations of the Terrestrial Ecosystem


Abiotic Inputs
Primary Producers
Herbivores (Primary Consumers)
Secondary Consumers
Decomposers

a. Simple


ATMOSPHERIC CO2
TULIP POPLAR
FOLIAGE FEEDERS
MISCELLANEOUS CANOPY SPECIES
R
R_s
GROUND COVER
UNDERSTORY SPECIES
STANDING DEADWOOD
FINE ROOTS
SOIL, LITTER AND DECOMPOSERS
R → RESPIRATION ABOVE-GROUND
R_s → RESPIRATION SOIL

b. More complex

Source: P. Sollins, Organic Matter Model and Budget for a Liriodendron Forest, Publication No. EDFB-IBP (Oak Ridge, Tennessee, Oak Ridge National Laboratory, 1971) pp. 72-73.

variable spatial and temporal distribution patterns determines the degree of accuracy with which a terrestrial ecosystem is represented.

Two important considerations in modeling terrestrial ecosystems are level of analysis and time. Quantitative analysis of terrestrial ecosystems can involve three distinct levels of analysis: (1) species level, i.e., individuals or population of like individuals; (2) trophic or food chain level, i.e., populations that depend on other populations as food resources; and (3) ecosystem level, i.e., all biotic populations considered. The level of analysis undertaken in any context depends on the questions to be answered regarding the ecosystem and on the extent to which field data are available or can be obtained. Obviously an ecosystem level analysis is practical only after sufficient information on individual species and on linkages between and among species has been obtained.

Although ecosystem components and pathways are constantly changing with time, most terrestrial ecosystem models only compare conditions at one point in time with conditions at another point in time. This type of analysis is termed state-of-the-system analysis. Such state-of-the-system terrestrial ecological models are analogous to the early aquatic ecosystem models. However, whereas the close relationship between aquatic ecological components and water body hydrology, as described in chapter 4, now enables iteration of state-of-the-system changes in short time intervals, no such "framework" exists for iterating state-of-the-system changes in terrestrial ecosystem models. Also, most rate functions[2] used in ecosystem level models are still only based on "annual averages," because of the complexity of this analysis level and costs of the associated data collection.

APPROACHES TO ANALYZING TERRESTRIAL ECOSYSTEMS

The two basic approaches used to analyze natural systems--statistical and conservation of mass and energy--were identified and described in the body of chapter 2. This section includes some comments with respect to the application of these approaches to analyzing terrestrial ecosystems.

Conservation of Mass and Energy Approach

Terrestrial ecosystem models based on the principles of conservation of mass and energy use balance equations for keeping track of the gains and losses for individual processes and components of a terrestrial ecosystem and for the system as a whole. Mass balances involving energy (kilocalories) and carbon predominate because of the basic photosynthesis connection, i.e., the conversion of light energy into organic molecules. Mass balances are also useful for keeping track of specific nutrients, such as essential metal ions, toxic metal ions, and other relatively long-lived substances such as pesticides and other man-made organic chemicals.

Terrestrial ecosystem models based on the conservation of mass and energy approach assume the processes which govern the movement of material and energy between components are nonstochastic. These processes are almost always nonlinear; hence, differential equations are required to represent them quantitatively. (In some contexts assumptions of linearity can be made.) For example, each of the pathways between components in figures 2-10a and 2-10b would be represented by a differential equation. All the equations would then be placed in a material/energy balance framework, using the principles of conservation of mass and energy. Ecological models based on conservation of mass and energy are referred to in the literature as process models or deterministic process models.

Because other types of NSMs are also based on the conservation of mass and energy approach, ecological models based on these principles can often be added to other NSMs. For example, the Terrestrial Ecosystem Hydrology Model (TEHM) (Patterson, et al., 1974) is representative of composite models formed by adding a terrestrial ecosystem model to a watershed runoff model. But because ecological processes are considered only indirectly to be computations of the hydrologic system, TEHM is basically considered a runoff model rather than a terrestrial ecosystem model. In order for TEHM to be considered a terrestrial ecosystem model, more extensive inclusion of biological processes would be required and the primary dependence on water movements to transport material and energy decreased.

Statistical Approach

Statistical methods have been widely used in analyzing terrestrial ecosystems. The essence of the approach is the determination of a statistically significant relationship between a dependent variable and a number of independent variables. The statistical method most often employed is regression analysis, although other methods have been applied (Parker and Armstrong, 1974).

The statistical approach is most commonly used to analyze portions of an ecosystem, e.g., at the species level of detail. An example is the analysis of the relationship between a characteristic of members of a species within a given community--e.g., volume increase in a tree species, fecundity in deer--and a number of environmental factors, or the relationship between one species and another species. The statistical approach is not applicable to analyzing ecosystems at the system level. Although analyses based on the statistical approach require lengthy data records, taken under rigidly controlled spatial and temporal patterns, they can be useful in developing preliminary ecological relationships from field data. The relationships or coefficients derived using the statistical approach usually become integral parts of the more complex process models based on conservation of mass and energy.

CURRENT STATUS OF TERRESTRIAL ECOSYSTEM MODELING

Very few NSMs of terrestrial ecosystems are operational at present (1979). This is true even for terrestrial ecosystems that have been exhaustively studied. In order to develop a comprehensive, system level, operational, terrestrial ecosystems model, it is necessary to integrate inputs from various subsystems into one functional model and then to test the outputs from that model against observed conditions. A major difficulty in developing system level models is that the more processes which are added to the model, the more nonlinear relationships must be incorporated. Incorporating nonlinear relationships greatly increases model data needs and computational problems.

An important series of terrestrial ecosystem modeling efforts was carried out in the various U.S. projects of the International Biological Program (IBP) during the early 1970s. These projects sought to develop models of various North American terrestrial ecosystems: deciduous forests, coniferous forests, prairie grasslands, desert, and tundra.[3] These modeling efforts produced a number of detailed process submodels and a few ecosystem level models that link together several process submodels, e.g., nutrient budgets, energy budgets, biomass budgets. However, the resulting models are almost exclusively research-oriented and are applicable for REQM analyses only under extremely limited conditions. Table 2-4 lists the more advanced U.S. IBP terrestrial ecosystem models. Any attempts to apply these models to areas outside of the original research sites are likely to encounter difficulties. Relatively few user's manuals are available for application under different REQM contexts. However, IBP project reports and model documentation reports often have unique theoretical descriptions of important terrestrial ecological processes and the modeling procedures needed to simulate them.[4] These can be helpful in considering the analysis of relevant terrestrial ecological systems in REQM analysis.

In contrast to these research-type terrestrial ecosystem models are management-oriented models developed to generate information for regional development and REQM decisions. Chapters 11, 12, 13, and 14 in Holling (1978) contain examples. Each of these examples was developed for a particular region and a specific decision context. Admittedly, the terrestrial ecosystem models developed are based on many simplifications, but the efforts indicate how the analysis of such systems can usefully be undertaken for REQM analyses.

Less sophisticated approaches can also be useful. In fact, a "full fledged" ecosystem level model may not even be required. Nutrient budget models, system-wide biomass models, and ecosystem energy models are examples of models of selected subprocesses. Models such as these can be used to address certain problems and provide useful information for REQM decisions.

Problems in Modeling Terrestrial Ecosystems

The status of terrestrial ecological system modeling can be more readily understood if some of the problems in such modeling are indicated.

Table 2-4. Research-oriented Ecosystem Process and Simulation Models Developed during the U.S. IBP Biome Projects

Biome Group	Model Acronym	Purpose	Reference
Desert	ANT	Harvester ant effects on plant seed dispersal	Desert Biome Modeling Group (1971a)
Desert	CAMEL	Competitive grazing by three large ungulates on five plant species	Desert Biome Modeling Group (1971b)
Desert	CAMP	Effects of campgrounds and associated activities on the desert environment	Desert Biome Modeling Group (1971c)
Desert	COYRAB	Interactions between vegetation, rabbits, and coyotes, esp. rabbit population dynamics	Desert Biome Modeling Group (1971d)
Desert	CREEK	Effects of hydrophilic vegetation on stream water balance	Desert Biome Modeling Group (1971e)
Desert	HOPPER	Grasshopper population dynamics	Desert Biome Modeling Group (1971f)
Desert	PANIC	Growth model for panicgrass	Desert Biome Modeling Group (1971g)
Desert	PLANT	Generalized desert plant growth model, including competition for light, water, nutrients under various grazing pressures	Desert Biome Modeling Group (1971h)
Desert	RANGE	Interaction of rabbits and rodents on grasses	Desert Biome Modeling Group (1971i)
Eastern Deciduous Forest	PROSPER	Hydrologic model of atmosphere-soil-plant water flow	Goldstein and Mankin, (1972); Goldstein Mankin, and Luxmoore, (1974); Swift, Swank, Mankin, Luxmoore, and Goldstein (1973)
Eastern Deciduous Forest	SERENDIPITY	Watershed level simulation model of tree biomass dynamics	Goldstein & Harris (1973)
Eastern Deciduous Forest	SIMCOT	Simulation model for cotton growth and yield	Duncan, Loomis, and Williams (1971)
Eastern Deciduous Forest	SPAM	Photosynthesis and microclimate predictions for crops and forest with a soil-plant-atmosphere model	Allen, Jensen, & Lemon (1971)
Eastern Deciduous Forest	TAEDA	Conceptual model of loblolly pine growth	Murphy & Hesketh (1972)
Eastern Deciduous Forest	TEEM	Terrestrial ecosystem energy model	Shugart, O'Neill, Goldstein, & Mankin (1974)
Grasslands	ELM	Ecosystem model for grasslands	Anway, et al. (1972)
Grasslands	GROMAX	Grassland community photosynthesis model	Connor (1973)
Grasslands	PWNEE	Complex grassland ecosystems model (Pawnee site)	Bledsoe, Francis, Schwartzman, & Gustafson (1970)
Tundra	ABISKO	Model for intersite comparisons of tundra decomposition process	Bunnell & Dowding (1972); (1973)
Tundra	METLEM-LEMPOP	Models for lemming growth, metabolism, and population dynamics	Collier, Stenseth, Osbourne, & Barkley (1974)
Tundra	TUNDRA	Ecosystems model for tundra	Bunnell (1972)

This section briefly discussed four major problems, the order of discussion not indicating order of importance.

The first is the inherent complexity of terrestrial ecosystems. Generally such systems are more complex than ecosystems in receiving water bodies (aquatic ecosystems) and hence more difficult to analyze. One factor is the greater number of interactions which take place on the land surface than in aquatic ecosystems. Whereas in aquatic ecosystems algae are the dominant primary producers and therefore can be treated as an homogeneous group, the variety of rooted plants in a terrestrial ecosystem, e.g., trees, shrubs, grasses, makes it difficult to generalize about terrestrial plant communities because of the different amounts of biomass different plants represent. Another factor contributing to complexity is comprised of the highly seasonal cycles of primary productivity, especially in temperate zones. These cycles are paralleled by abundant changes in local animal populations. In fact, many mammal and bird populations considered to be important indicators of AEQ are transient, e.g., migrate in and out of territory in many areas. Fish and other aquatic organisms follow analogous patterns, but their movements are confined by the actual boundaries of the water body. Only in estuaries and coastal waters can aquatic organisms migrate into and out of a "region" relatively freely.

An important implication of ecosystem complexity is its effect on model calibration and verification. Because the problems which terrestrial ecosystem models are intended to analyze are, typically, caused by both intentional and unintentional alterations that are occurring simultaneously, it is very difficult--often impossible--to calibrate and verify models against observed phenomena. It is rare that sufficient data can be obtained to enable both calibration and verification to be accomplished for a given model in a given region.

A second major problem is the establishment of appropriate analysis boundaries for any given terrestrial ecosystem and the effects of the boundaries on data requirements and model outputs. When a terrestrial ecosystem model is based on conservation of mass and energy, the establishment of a control volume--the defined volume in which the processes are to be modeled--is required to quantify ecosystem transfers and storage of material and energy. A control volume establishes boundaries in all directions so that a mass or energy balance can be performed for the appropriate system.

Establishing control volumes for terrestrial ecosystems is more difficult than for aquatic ecosystems. Whereas boundaries for a control volume for an aquatic ecosystem such as a receiving water body can be established using easily recognizable physical boundaries, e.g., shorelines, streambed, stream banks, water surface, establishing boundaries for a terrestrial ecosystem is considerably more arbitrary. Terrestrial ecosystem boundaries may be set to include a particular forest stand, plant community, land use category, watershed, or other physiographic areas. Boundaries for most terrestrial ecosystem models tend to follow watershed boundaries or actual spatial patterns of the dominant vegetation within small internal subdivisions. However, the smaller the size of the spatial units the greater the data requirements. Also, depending on the group of organisms considered--primary producers, secondary producers, decomposers--boundaries are more or less difficult to establish. For instance, primary producers tend to be spatially invariant and therefore can be studied on a community basis as well as on a small spatial unit basis. In contrast, secondary producers, e.g., animal consumers, are highly spatially and temporally variable. Hence, when secondary production is considered, boundaries are more difficult to establish.

A third major problem is the lack of understanding of the effects of, and the inability to model, the impacts of toxic materials on terrestrial ecosystems. Toxic, nondegradable substances such as heavy metals and pesticides are the primary residuals of concern in terrestrial ecosystems. Residuals such as sediment, nutrients, organic matter, and pathogenic bacteria which are so important in aquatic ecosystems are generally innocuous or even beneficial to terrestrial ecosystems. Toxic substances can be and often are biomagnified within the food chain, so that the impacts are distributed among a variety of species.

A fourth major problem involves the fact that most terrestrial ecosystems are substantially affected by fires occurring at varying points in time. Fire--whether a result of natural or human causes--represents a major energy transformation in such systems, which transformation can greatly alter the ecosystem. The direction of alteration may be positive or negative, both through immediate direct effects, e.g., removal of certain species, and through indirect effects, e.g., increasing susceptibility to mass wasting and water-induced erosion.

CONCLUDING COMMENT

As stated above, very few, if any, models of terrestrial ecosystems are operational in the sense defined in this report. This is contrary to the other categories of natural systems models discussed herein: runoff from land surfaces; receiving water systems; and atmospheric systems. Therefore, in all REQM contexts in which information is required regarding terrestrial ecosystems, it is quite likely that experts will have to be consulted with respect to the types of analyses which are possible to undertake and the associated resources required, e.g., time, data, personnel. Despite the inherent difficulties of representing terrestrial ecosystems with mathematical models, such models, if operated with full knowledge of their limitations, can provide useful insights for REQM analysis.

NOTES

[1] Primary production is defined as the organic matter produced by mixed communities of trees, shrubs, grasses, and other plants within a given terrestrial ecosystem. This output serves as the source of energy and material for diverse populations of animals and microbial decomposers. Plants, from microscopic algae to giant trees, utilize light-sensitive pigment which can capture radiant energy and convert it biochemically into stored energy in the form of organic compounds. This process, known as photosynthesis, requires inputs of solar radiation, water, carbon dioxide, and soil nutrients, i.e., various forms of nitrogen, phosphorus, and trace metals.

Secondary production is defined as the sum total of all animal consumer biomass within a given terrestrial ecosystem, including all herbivores (animals which consumer plants), carnivores (animals which consume other animals), and omnivores (animals which consume both plants and animals).

Decomposers, i.e., microbial organisms, derive their basic inputs from the decay and breakdown of wood, leaf, litter, organic detritus fragments, animal carcasses, and animal wastes. Both secondary production consumers and decomposers utilize the process of respiration to convert the energy stored in organic matter into biologically useful forms of energy.

[2] A rate function is the quantity of material or energy transferred per unit of time between components of an ecosystem.

[3] Primary IBP research centers were the Oak Ridge National Laboratory for the Deciduous Forest Biome, Utah State University for the Desert Biome, University of Washington for the Tundra Biome, Oregon State University for the Coniferous Forest Biome, and Colorado State University for the Grassland Biome.

[4] Many of the terrestrial ecosystem models developed under the IBP projects have remained underpublished or unpublished, because of inappropriate format or too lengthy discussions of the model building process.

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Chapter Three

ANALYZING RESIDUALS GENERATION AND DISCHARGE FROM URBAN AND NONURBAN LAND SURFACES

Wayne C. Huber and James P. Heaney

INTRODUCTION

Residuals generation on and discharge from land surfaces is primarily the result of the action of precipitation on and the subsequent movement of water over the land surface. In some cases residuals generation and discharge is the result of water applied to land by man for agricultural purposes. The quantity of residuals generated and discharged from an irrigated area depends on the manner in which the water is applied, e.g., method of irrigation (ditch and border check, furrow, spray), and the way in which irrigation is managed (frequency, duration, and intensity of application). In all cases, residuals discharges from land surfaces eventually reach receiving water bodies. This type of residuals generation and discharge is most commonly referred to as nonpoint pollution; another term which is also used is dispersed pollution. To be consistent, through this chapter and this report the term nonpoint sources of residuals generation and discharge is used.

All land use activities are nonpoint sources of residuals generation

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Authors' note: A glossary of terms can be found at the end of the chapter.

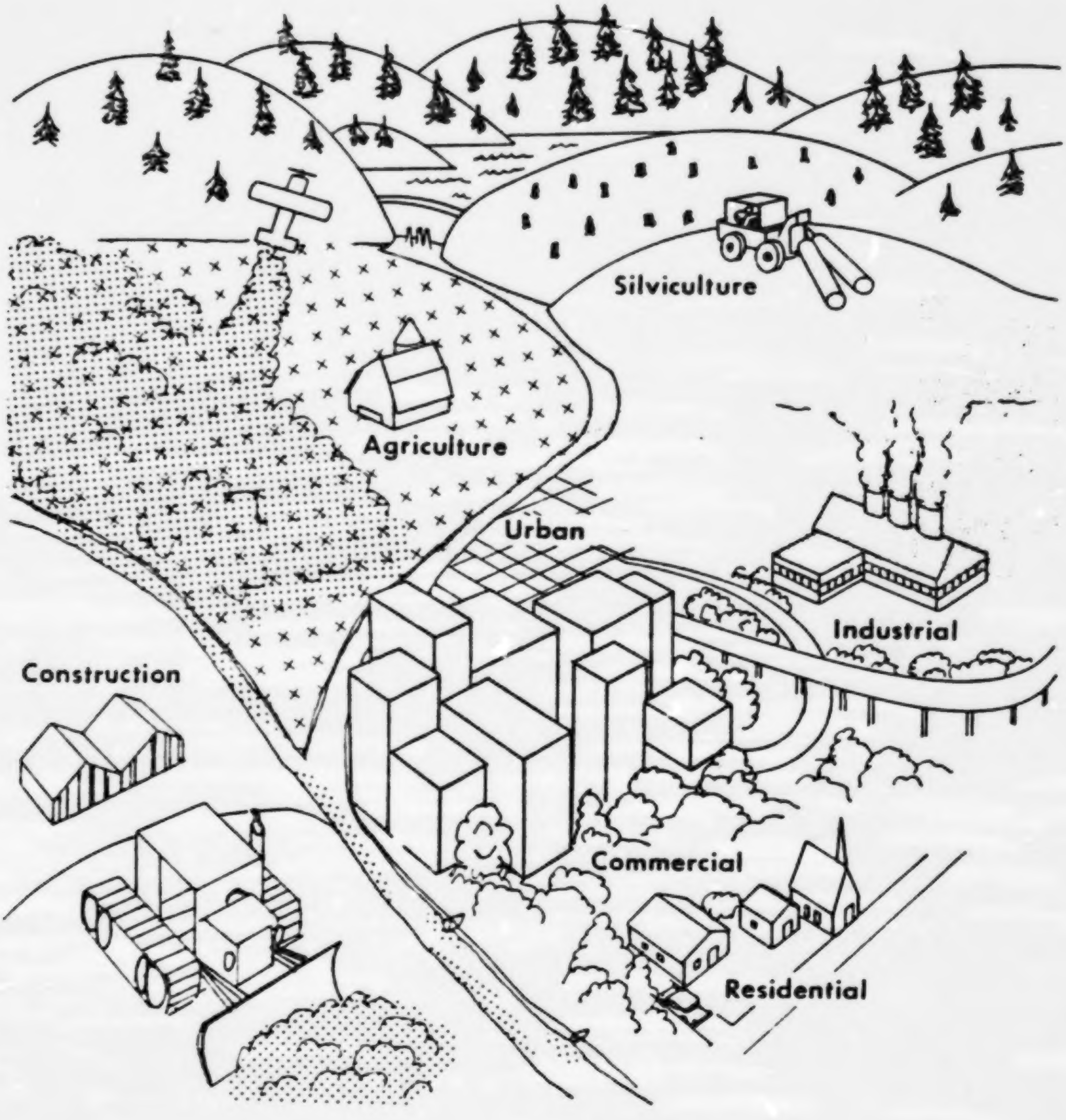
and discharge. Figure 3-1 illustrates a mix of land use activities that might exist in any given region. Depending on the type of activity occupying a parcel of land, the amount of water which will move over the land surface and the amounts and types of residuals carried with it will vary. The amount of water which moves over the land surface and eventually enters a receiving water body is the difference between the amount of water which either falls on or is applied to the land and the amount which is absorbed by, evaporated and transpired from, and/or stored on the land in depressions, ditches, and puddles. The intensity and duration of precipitation and the time since the last precipitation event also affect the quantity of residuals generated and discharged. These and other factors are discussed later in the chapter.

Natural systems models (NSMs) which analyze nonpoint sources of residuals generation and discharge are commonly referred to as "runoff models." For convenience, this term is used throughout the chapter. Operationally, runoff models are defined as NSMs which estimate the temporal and spatial distribution of water and associated residuals that run off the land surface due to precipitation, and enter receiving water bodies.

The purpose of the chapter is to assist individuals in selecting a runoff model for analyzing residuals generation and discharge from the land surface in various REQM contexts. The chapter is organized into four sections to facilitate this process.

The first section identifies and describes briefly the major problems associated with residuals generation and discharge from the land surface. Note that the ambient water quality problems which result when residuals discharges from land surfaces (nonpoint sources) enter receiving water bodies are not discussed in this section. Receiving water problems that

Figure 3-1. Nonpoint Sources of Residuals Generation and Discharge


Silviculture
Agriculture
Urban
Industrial
Construction
Commercial
Residential

Source: A. S. Donigian, Jr., and N. H. Crawford, Modeling Nonpoint Pollution from the Land Surface, Report No. EPA-600/3-76-083 (Athens, Georgia, U.S. Environmental Protection Agency, 1976).

result from residuals inputs from all sources, nonpoint sources included, are discussed in the next chapter. This section focuses on describing briefly the operational distinction between the quantity and quality aspects of nonpoint source residuals discharges and how these aspects have stimulated development of runoff NSMs.

The second section identifies and describes the natural processes which affect the movement of water and related transport of residuals over the land surface. In order to estimate the spatial and temporal distribution of residuals discharges from nonpoint sources, these processes must somehow be taken into account. Hence it is important to give some explanation of these processes. To a large extent, these processes are the same as those which are described in the next chapter. This is particularly true in cases where overland flow is directed into and flows in channels, as in storm sewers in urban areas, before entering receiving waters. The physical processes affecting flow in channels carrying runoff are analogous to those affecting flow in a receiving water body such as a stream or river. Because of the obvious overlap with the next chapter, this section provides additional description only in cases where a process either has a significantly different effect or is treated differently in the analytical process.

The third section describes the basic approaches used to formulate runoff models. This section builds upon the related section in chapter 2 describing how the approaches to analyzing natural systems explained in chapter 2 are modified for analyzing runoff.

The fourth section describes how to select a runoff model for any given context. This section relates directly to the section in chapter 2 on setting up the analysis of natural systems. Four elements comprise this section: (1) a listing of a large number of runoff models, both operational and nonoperational, characterized as the population table; (2) a table which relates characteristics of problem contexts to operational runoff models, the problem table; (3) a flow diagram which indicates how to select a runoff model given the material in the chapter, the selection procedure; and (4) a discussion of the characteristics used to summarize the operational runoff models contained in Appendix A.

Appendix A contains detailed summary tables for fourteen operational runoff models. Appendix B contains a list of annotated references for each of the fourteen runoff models summarized. References for runoff models included in the population table, but not considered to be operational at this time, are included in the general list of references at the end of the chapter.

MAJOR PROBLEMS

The effects of precipitation on the land surface and the resultant movement of water and material off the land, eventually being deposited partially or fully in receiving waters, can be separated into two interrelated problems. The first, the primary focus of REQM is the effect on ambient receiving water quality of the addition of residuals washed off the land surface, the quality aspect. The second is the effect of man's use of water and man's activities on the volume of water which runs off the land surface, the quantity aspect. Of course, the quality and quantity aspects can never be totally separated. But the distinction is operational, both in terms of identifying typical problems and explaining analytical approaches.

A third problem, a corollary to the quantity/quality aspects, is the effect of the overland flow of water and removal of material on the quality of land, i.e., state-of-the-system. Examples are the effects on agricultural productivity of soil erosion and of increased soil salinity due to irrigation. This problem is mentioned to indicate the full range of impacts of residuals discharges from the land surface, and because much of the initial stimulus for analyzing residuals in runoff stemmed from concern for reducing soil erosion to maintain productivity of agricultural lands, rather than concern for improving the ambient quality of water bodies. In order to assess the impacts of runoff on land quality, NSMs are needed which relate the effects on terrestrial ecosystems to precipitation on the land and to the materials--soil particles, fertilizers, pesticides--consequently removed. Such NSMs are known as terrestrial ecosystem models, and are discussed in Appendix B of chapter 2.

It is the recognition of the problems cited above which, over time, has stimulated the development and refinement of runoff models for analyzing residuals generation and discharge from land surfaces. The discussion which follows briefly describes the quantity and quality aspects of runoff and the types of model development these aspects have stimulated.

Two definitions are necessary before proceeding. Urban and nonurban are terms commonly used as descriptors of types of runoff, e.g., urban runoff and nonurban runoff. Urban runoff refers to runoff from areas of relatively high population density, areas which are relatively impervious--do not absorb water--because of the amount of land area covered by roads, sidewalks, parking lots, and buildings. Nonurban runoff refers to runoff from all land areas other than urban. Nonurban includes many types of land use activities such as: park land; agricultural land in crops; orchards or pasture; range land; forest land; mining areas. These varied activities result in very different patterns of runoff in terms of quantity, quality, and time pattern. Despite the range of land use types included in nonurban, the terminology does have some utility in relation to distinguishing between types of runoff models. Models developed to estimate residuals discharges from urban areas differ from models developed to estimate residuals discharges from nonurban areas. For example, models of urban areas must include consideration of factors such as street gutters, sewers, roof top storage, which nonurban models do not have to take into consideration.

Quantity Problems

Problems relating solely to the quantity of water and the tools used to analyze them are not of primary concern in REQM, although such problems are important in their own right in certain contexts. However, some discussion of "purely" quantity problems is warranted as a basis for understanding the quality problems.

A large number of problems exist which can be termed water quantity problems, the majority of which are explained in any number of standard hydrology textbooks, e.g., Chow (1964). The two most important are flooding and water supply.

Flooding affects all land use activities located in flood plains, both urban and nonurban. Problems associated with flooding have stimulated the development of analytical tools for the prediction of flood magnitudes (flows), flood stages (heights), flood volumes, and flood durations, and for the design of measures for modifying flood flows and for adjusting to flood flows. In an urban area, for example, a drainage network consisting of gutters, pipes, channels, comprises a set of facilities designed to remove stormwater and reduce flooding. Such a system would be designed based on an assumed storm condition, e.g., a ten-year return period storm. Some recently formulated urban runoff models now enable analysis of very complex hydraulic problems such as surcharging and basement flooding. Although flood problems have been analyzed for centuries, analytical techniques continue to be improved for applications in both urban and nonurban areas.

Water supply problems relate to the time pattern of flow available for various types of water uses, e.g., industrial, residential, irrigation, fisheries, and hence to the design of supply facilities, e.g., reservoirs, wells, pipelines, pumping plants, distribution systems. In connection with these problems, especially useful models have been developed for simulation of long-term streamflow records for use in deciding on capacities of such facilities as reservoirs, pipelines, and pumping plants.

Advances in mathematical techniques and computer hardware and software now enable models to be used in solving operational problems in hydrologic networks. In nonurban areas, flood forecasting methods are used to aid the selection of spillway capacities and the operation of diversion channels. In urban areas, with much shorter response times, software is just now at a point at which limited automation of the operation of weirs, pumps, and combined sewer overflow regulators is possible.

Quality Problems

Quality problems relate to the ambient quality of receiving water bodies, not to the ambient concentrations of residuals in water as it moves over the land surface, in conduits, and in channels on its way to a receiving water body.[1] Chapter 4 describes the major water quality problems with respect to receiving water bodies: temperature, salinity, sedimentation, dissolved oxygen, eutrophication, toxic substances, and biological effects. Depending on the context, including type of water body and geographical locale, residuals from nonpoint sources contribute to all ambient water quality problems to a greater or lesser extent. Thus, the main objective of analyzing runoff from land surfaces is to determine inputs of residuals to receiving waters.

The extent to which residuals discharges from nonpoint sources affect water quality, in any context, depends upon the intensity and time pattern of the discharge. There is a continuum of intensity-time patterns of residuals discharges from nonpoint sources and an accompanying continuum of related water quality effects. One end of the continuum is an intensity-time pattern of discharge in which, although the magnitude of residuals entering a receiving water body is large relative to other sources of residuals during a given time period (the duration of a storm runoff), the residuals do not overpower living organisms in the short-run, e.g., cause fish kills. Residuals from nonpoint sources entering receiving water bodies in such intensity-time patterns do contribute to longer-run water quality problems, such as increased eutrophication due to nutrients (fertilizers) washed off agricultural lands, increased concentrations of toxic substances because of inputs of toxic materials washed off urban streets, and the filling in of impoundments over time by sediment from land surface erosion induced by precipitation and the subsequent transport of sediment by overland flow of water.

The other end of the continuum is an intensity-time pattern of discharge in which the magnitude of residuals entering a receiving water body during a given time period has an overpowering effect in the short-run and seriously damages the existing ecosystem. An example is the so-called "flash flood," where heavy sediment loads entering a water body choke fish and scour benthic deposits, killing benthic organisms.

The intensity-time patterns of residuals discharges from nonpoint sources and their related effects on water quality are important because it is the recognition of these patterns which has conditioned the development of runoff models and their use in conjunction with receiving water NSMs in analysis for REQM. As more has become known of these patterns and their effects on ambient water quality, runoff models have become more complex in order to account for the dynamic characteristics of residuals discharges. For example, this recognition is reflected in the development of nonsteady state receiving water models capable of analyzing the effects of time-varying residuals discharges from nonpoint sources.

Although water quality problems resulting from nonpoint sources of residuals discharges are most frequently related to problems of erosion and sedimentation, runoff models often include consideration of other residuals as well, such as biochemical oxygen demand (BOD), organic material, nitrogen (N), phosphorus (P), bacteria, metals, pesticides, and many forms of "solids."[2] Chlorides are sometimes considered because of problems associated with highway de-icing chemicals (Field, et al., 1973). Characterization of residuals discharges associated with various types of land uses can be found in many sources. For example, the results of several studies are summarized in Environmental Protection Agency (1973). For residuals discharges associated specifically with urban areas, see Lager, et al. (1977).

Summary Comments

The linkages between the quantity and quality aspects of runoff from land surfaces should be emphasized for at least two reasons. First, in most water quality models, foreknowledge of the quantity aspects is a requirement. (The exceptions are mainly with respect to some statistical approaches for residuals generation on land surfaces.) Thus, concentrations and loads cannot be estimated without having estimated flows. It is for this reason that all but two of the fourteen water quality models described in detail in the model summary tables of this chapter include hydrologic simulation capabilities of varying degrees of complexity. Second, procedures to mitigate quantity and quality problems are often complementary. Thus, a retention basin operates to reduce flood peaks as well as serving as a sedimentation basin to reduce sediment discharges downstream.

MAJOR NATURAL PROCESSES

Water and accompanying residuals are discharged from land surfaces as the result of naturally occurring processes, except in irrigation, where water is applied to land by man. But even in the case of irrigation, all processes affecting runoff, other than the application of water, are natural processes. Modifications which man has made to the land surface have exacerbated these processes in many regions, thereby increasing the quantity of residuals discharged and altering both the types of residuals and the time patterns of discharges. Consequently, in order to estimate the quantity and quality of water which runs off any given land surface, these processes must somehow be taken into consideration.

The extent to which runoff models explicitly take these processes into account varies from model to model. Purely statistical models ignore explicit consideration of most of these processes altogether. Therefore, it is important that some explanation of the natural processes affecting runoff be provided as background for selecting an appropriate runoff model and for interpreting the results of the model after it has been applied.

Five natural processes affect the movement of water and residuals over the land surface and in conveyance systems and the related transformations of residuals. These are: physical processes, also termed physical transport processes; chemical processes; physicochemical processes; biochemical processes; and ecological processes. This section explains aspects of these processes which are especially important with respect to runoff. Additional descriptive material relating to these processes is in chapter 4.

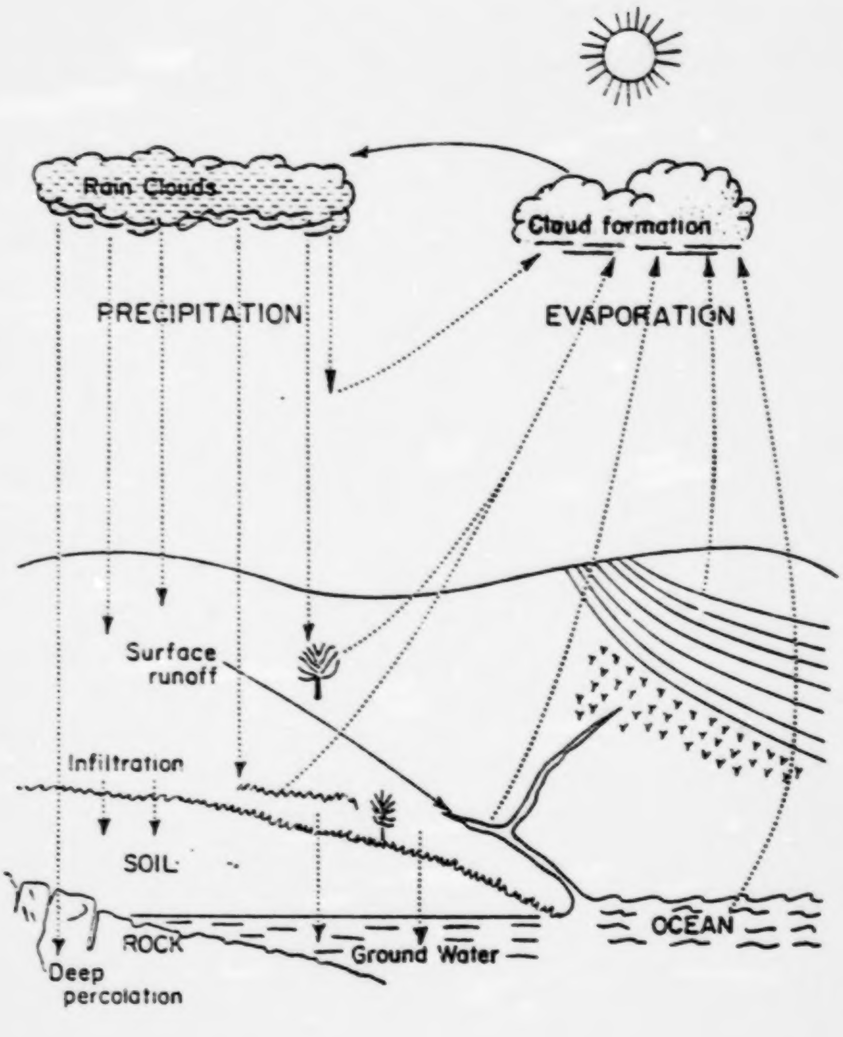
Physical Processes

In relation to runoff from land surfaces, physical transport processes are those processes which affect the movement of water, and the movement of materials in water, over the land surface, and in conveyance systems, e.g., pipes, canals, channels, ditches, before entering receiving water bodies.

The net amount of water which runs off the land surface is a function of many factors, all of which are embodied in one way or another in the hydrologic cycle, depicted in figure 3-2. The hydrologic cycle is defined as the circuit of water movement from the atmosphere to the earth and its return to the atmosphere through various processes.

The hydrologic cycle begins with precipitation. Precipitation in the form of rain falling on the land surface is subject to initial losses due to interception by vegetation and the filling of small pores and depressions on the land surface. The amount of water intercepted in this fashion

Figure 3-2. The Hydrologic Cycle


Rain Clouds
Cloud formation
PRECIPITATION
EVAPORATION
Surface runoff
Infiltration
SOIL
ROCK
Ground Water
OCEAN
Deep percolation

Source: J. C. I. Dooge, Linear Theory of Hydrologic Systems, Technical Bulletin No. 1468, U. S. Department of Agriculture, (Washington, D.C., U.S. Government Printing Office, 1973).

is termed depression storage. Water which is lost to depression storage is assumed to evaporate back to the atmosphere. The quantity of rainfall which exceeds depression storage is available for infiltration into the land surface (through pervious areas) or for overland flow (sheet flow) toward small stream channels.

Water which infiltrates the land surface may fill up available storage in the zone of aeration (also termed the unsaturated zone) or move by gravity into the zone of saturation, commonly referred to as the "water table." Water movement in the zone of saturation is governed by the principles of flow through porous media. [See Bear (1972).] Water may also move through the zone of saturation into deeper groundwater zones and effectively disappear from a region. Subsurface water can also move laterally through the soil and enter surface water bodies. Water which has infiltrated the land surface and moves into surface water bodies without first reaching the zone of saturation is called interflow.

When precipitation falls on the land surface in the form of snow, runoff does not occur until the snow begins to melt. Runoff due to snowmelt is a major component of the hydrologic cycle in many areas. In order to estimate runoff from snowmelt, the "thermodynamics" of the melting process must be considered. For runoff to occur, sufficient heat must be added to the snow pack to raise its temperature to 0° C and then to provide the latent heat of fusion, 80 cal/g, necessary to melt the ice crystals. A snowpack can receive heat inputs via solar radiation (short wave radiation), atmospheric radiation (long wave radiation), conduction of heat from the atmosphere, latent heat from the condensation of water vapor, advection of heat by rainfall, and conduction of heat through the ground. Losses of heat can occur via long wave radiation, conduction to the atmosphere and ground, and sublimation. After runoff begins, the movement of water over and through the land surface is as described above.

Even though the hydrologic cycle is the starting point of any analysis of runoff, the extent to which models include specific aspects of the cycle varies. In many models simplifying assumptions are adopted. For example, many runoff models developed for urban areas do not include subsurface hydrologic processes. The assumption made is that because a high percentage of land surface in urban areas is impervious, only negligible quantities of water infiltrate the surface and contribute to subsurface flows. Accurate representation of the hydrologic cycle is a prerequisite for accurate estimation of runoff.

Once runoff begins, the velocities and directions with which water moves over the land surface and in conveyance systems are a function of the intensity and duration of precipitation and the physical characteristics and geometry of the land surface and of conveyance systems. Characteristics not already mentioned include: slope; composition of strata; configuration of conveyance channels, e.g., depth, slide slopes, length, and surface roughness; and barriers to flow. This movement of water is governed by the fundamental laws of conservation of momentum and conservation of mass and energy. These laws may be coupled in various ways to provide a set of "motion equations" to describe the movement of runoff water. [See Daily and Harleman (1966) and Henderson (1966).] The portion of a runoff model which describes the movement of water is analogous to the hydraulic block in a receiving water model, as described in chapter 4.

Runoff "picks up" residuals by either dissolving material which has accumulated on the land surface or physically suspending the material and carrying it along. As water begins to accelerate over the land surface (bed), hydrodynamic forces of lift and drag begin to act on individual particles with greater and greater force. Particles will first roll and slide along the bed and then move with short jumps, returning to the bed for variable periods of time. Material which rolls and slides along the bed is termed contact load; if the material remains in contact with the bed as it moves it is termed bed load. Material which continues to move in short jumps is termed saltation load. As water velocity increases further, more frequent jumps occur and some material remains suspended for long periods of time due to turbulence. Such material is termed suspended load. Material which tends to remain suspended and seldom comes in contact with the bed, e.g., clay particles, is termed washload. The term sediment is usually used to refer to solid materials which are moved by water. The combination of materials and processes described above is referred to as the sediment transport process.

It is important to emphasize that what constitutes sediment is poorly defined. Many varied residuals may be present in any so-called sediment load, either as solid particles or attached to solid particles. Methods which can analyze accurately the total sediment transport process are not yet available. However, the following factors are known to influence the process: particle size, shape, specific gravity; particle concentration; temperature, viscosity, density; flow velocity, distribution of velocity, turbulence; surface roughness; and channel shape.

The movement of residuals within runoff water is affected by two fundamental processes: advection and diffusion. Both processes have been defined and described in chapter 2. Because these processes have the same effect on the movement of residuals in water, regardless of whether the water is runoff in a conduit or flow in a stream, no additional discussion of these processes is presented.[3]

A physical process not previously mentioned, but which is important with respect to residuals generation and discharge from land surfaces, is solids accumulation. Solids accumulation occurs from dust fall or dry deposition, wind and water erosion, and a variety of man-made sources. Some of the materials may have been transported hundreds of miles. Solids accumulation is an important process because it affects the quantity of residuals available to be picked up by runoff.

Analyzing interactions among solids, water, and wind is considerably more complicated than analyzing interactions between only solids and water (Vanoni, 1975). Even so, theories of sediment transport are seldom used to analyze the washoff of residuals from land surfaces, because of the complexities of water-solid interactions. As indicated earlier, no accurate analytical representations of the total sediment transport process are presently available. Analyses are most often carried out using coefficients based on either empirical formulations or statistical analyses, e.g., regression analysis. An example of such analysis is the Universal Soil Loss Equation (Wischmeier and Smith, 1965). This equation is briefly explained in the section on analytical approaches.

An important phenomenon relating to solids accumulation and to residuals generation and discharge from land surfaces is the first flush effect. The first flush effect relates to the high concentrations of residuals, especially solids, which often occur in the early portion of a runoff event. The first flush effect occurs in both urban and nonurban areas. In urban areas, material which has accumulated on the surface during dry weather conditions, and material which has previously been deposited in channels and pipes and is "scoured" out by high velocity and turbulent runoff waters, are the primary causes of the first flush effect. The analogous phenomenon of accumulation of material on land surfaces and on vegetation occurs in nonurban areas.

Chemical, Physicochemical, and Biochemical Processes

Physical processes associated with runoff account only for the movement of conservative and nonconservative residuals within water, and have little or no effect on the transformations of nonconservative materials which take place.[4] The transformations which do occur are the result of reactions caused by chemical, physicochemical, and biochemical processes. However, because of the short period of time for rainfall to wash residuals off land surfaces, little or no transformation occurs before residuals are discharged into receiving waters or into holding basins from which discharge eventually occurs into receiving waters. The extent of transformation which occurs during runoff is usually negligible in relation to the transformation which occurs in a receiving water body or in a holding basin. Consequently, very few runoff models explicitly consider chemical and biochemical processes. Runoff models which do include chemical and biochemical processes typically consider travel times on the order of a few hours or consider storage basins as part of the conveyance system, or both. Chapter 4 describes how chemical and biochemical processes affect residuals transformations in water.

Physicochemical processes, on the other hand, have an important effect on ambient concentrations of residuals in runoff, regardless of the short time frame involved. The most important physicochemical processes are adsorption/desorption and absorption. Adsorption is the adhesion of a substance to the surface of a solid or liquid. Adsorption is an important process because many residuals, e.g., nitrogen, phosphorus, various pesticides, and heavy metals, attach themselves to sediment particles and are in turn transported with the particles in runoff. The quantities of residuals which become attached to sediment particles are a function of the concentration of residuals in the runoff stream and temperature (Metcalf and Eddy, 1972). Desorption is when the adsorption process is reversed, i.e., the residuals are detached from the sediment particles. Absorption is the penetration of a substance into or through another substance. Absorption usually takes place at the air-water interface where gases, e.g., oxygen, are absorbed into water. Although a certain amount of absorption does take place during runoff, the overall effect is negligible compared to the residuals collected off the land surface and carried in the runoff.

Ecological Processes

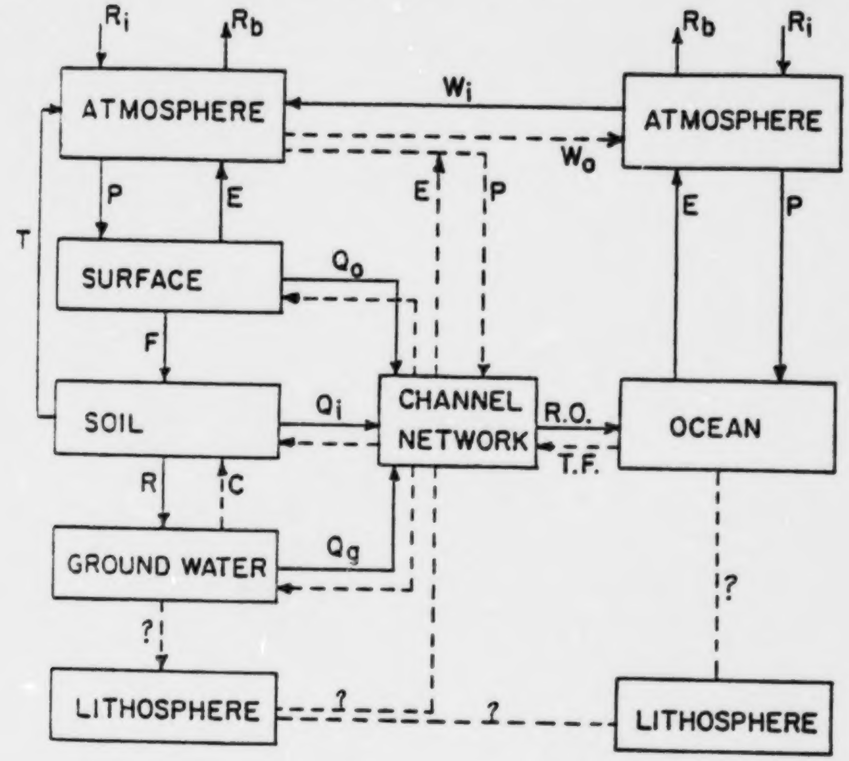
Ecological processes relate to the linkages between and among living organisms. These linkages typically involve the consumption of one species or organism by another which is higher in the food chain, and the consumption of that species by another, and so on. An example of an ecological process--or set of processes--which can affect runoff is an alteration of the predator-prey relationship such that overgrazing of one or more species of vegetation takes place. Because less vegetative cover is available to absorb the impact of raindrops, to hold soil, and to transpire water, both runoff and the amount of sediment in the runoff are increased. Although some ecological processes do have an effect on residuals discharges from the land surface, such processes are not considered in runoff models.

APPROACHES FOR ANALYZING RESIDUALS GENERATION AND DISCHARGE FROM THE LAND SURFACE

This section is organized differently than the sections on analytical approaches in the following chapters for two reasons. First, some of the methods which have been developed and used extensively over the years to estimate runoff volumes--the quantity aspect--do not fit neatly into the two categories of approaches for analyzing natural systems used throughout this report, i.e., statistical and conservation of mass and energy. Second, it is useful to maintain the distinction between the quantity and quality aspects when discussing approaches for analyzing runoff. This section, therefore, is organized into two parts: (1) approaches for estimating runoff volume; and (2) approaches for estimating runoff quality. The part on quantity estimation discusses the rational method and the hydrograph approach--two much used approaches--and the statistical and conservation of mass and energy approaches. The part on quality estimation discusses the statistical and conservation of mass and energy approaches.

Because all analyses of residuals generation and discharge from the land surface must somehow consider the various componetns of the hydrologic cycle, some generalizations can be made regarding the various approaches. Analytically, the hydrologic cycle can be represented as a series of interconnected boxes, as shown in figure 3-3. In order to estimate the quantity of water which runs off a given land surface in any given time period, the quantities of water moving between any two boxes and the amounts stored in each box must be mathematically represented. To estimate the quality of the water, residuals generation in each box and transport between any two

Figure 3-3. Block Diagram of the Hydrologic Cycle


R i
R b
R b
R i
ATMOSPHERE
W i
ATMOSPHERE
W o
P
E
E
P
E
P
T
SURFACE
Q o
F
SOIL
Q i
CHANNEL NETWORK
R.O.
OCEAN
T.F.
R
C
GROUND WATER
Q g
?
?
LITHOSPHERE
?
?
LITHOSPHERE

Flows are identified as follows:

P = Precipitation

E = Evaporation

T = Transpiration

F = Infiltration

R = Groundwater Recharge

C = Groundwater Seepage

Q_o = Surface Runoff (e.g., Overland Flow)

Q_i = Interflow

Q_g = Groundwater Runoff

R.O. = Channelized Runoff

T.F. = Tidal Flow

W_i, W_o = Wind Fluxes of Moisture

R_i = Incident (Solar) Radiation

R_b = Back (Terrestrial and Atmospheric) Radiation

Source: J. C. I. Dooge, Linear Theory of Hydrologic Systems, Technical Bulletin No. 1468, U.S. Department of Agriculture (Washington, D.C., U.S. Government Printing Office, 1973).

boxes must be analyzed in conjunction with estimating quantity. Note that the "channel network" box in figure 3-3 represents both natural channels, i.e., streams and rivers, and man-made channels, such as storm sewers and drainage channels in urban areas.

Central to all approaches to analyzing runoff is the concept of a catchment or drainage area. A catchment is the area tributary to a surface water body. All runoff from precipitation on a given catchment drains into the related water body. The scale with which a catchment may be defined varies. A catchment can be as large as an entire agricultural region or metropolitan area, or it can be as small as an individual field or city block. Once an overall catchment has been defined, it can be subdivided into smaller subcatchments for more detailed analysis. Regardless of the analytical approach employed, the boundaries of the land surface to be studied must be established according to catchment boundaries.

One important difference among runoff models is the amount of detail with which catchments are analyzed. Some models use a "coarse" representation and treat the entire area as one or possibly two catchments. In these models internal pathways between any two subcatchments are only implicitly considered, while other models allow explicit consideration of all major pathways among numerous subcatchments within a given area.

Generalizations can also be made about differences in the ways quantity and quality aspects are handled in urban and nonurban runoff models. Regarding quantity aspects, three generalizations are relevant. The first involves the relative importance of various components of the hydrologic cycle in urban and nonurban settings. Usually more attention is devoted to subsurface flow routing and storage, pathways Q_i and Q_g in figure 3-3, in nonurban runoff models than in urban runoff models, because these are major pathways in nonurban areas. In contrast, in urban runoff models major emphasis is devoted to surface or overland flow, pathway Q_o in figure 3-3, and little or no attention to subsurface processes because of the large amounts of impervious areas in urban areas.

Second, the hydraulics of urban drainage systems are more complicated than those of nonurban systems. For example, phenomena such as backwater, looped connections, surcharging, and pressure flow--all important in urban drainage systems--are rarely important in nonurban systems. Hence, analysis of flows is usually more complicated in urban runoff models than in nonurban runoff models.

Third, response times of nonurban catchments tend to be considerably longer than those of urban catchments of the same size. (Response time relates to the amount of time it takes for precipitation to result in runoff from the land surface.) Hence, longer time steps are usually employed in nonurban runoff model computations than in urban runoff models. Conequently, input data such as precipitation records usually do not have to be delineated in as small time intervals for analysis of nonurban runoff as for analysis of urban runoff.

Regarding quality aspects, two generalizations are relevant. First, because flow velocities in urban catchments are faster due to shorter response times, impacts of chemical and biochemical processes on urban runoff quality are usually negligible, except in cases where storage and modification take place. Hence, these processes are omitted in most urban runoff models, but are taken explicitly into account in some nonurban runoff models, depending on the residual under consideration. Second, because nonurban land surfaces are relatively pervious, interactions between residuals and soil particles--with respect to both overland flow and subsurface flow--are more relevant to nonurban runoff models than to urban runoff models.

Most of the analytical approaches discussed below may be applied to all levels of scale and to both urban and nonurban areas.[5] References are provided relating to several kinds of applications for each analytical approach. Background information on analyzing residuals generation and discharge from land surfaces is available in many texts and reports. Eagleson (1970) presents a thorough discussion of the physics and thermodynamics of most hydrologic processes. A broad survey of engineering methods is included in such sources as Viessman, et al. (1977), and Linsley, Kohler, and Paulhus (1949). The texts by Overton and Meadows (1976) and Fleming (1975) are specifically devoted to hydrologic modeling. An excellent summary of several specific approaches discussed below is given by Dooge (1973).

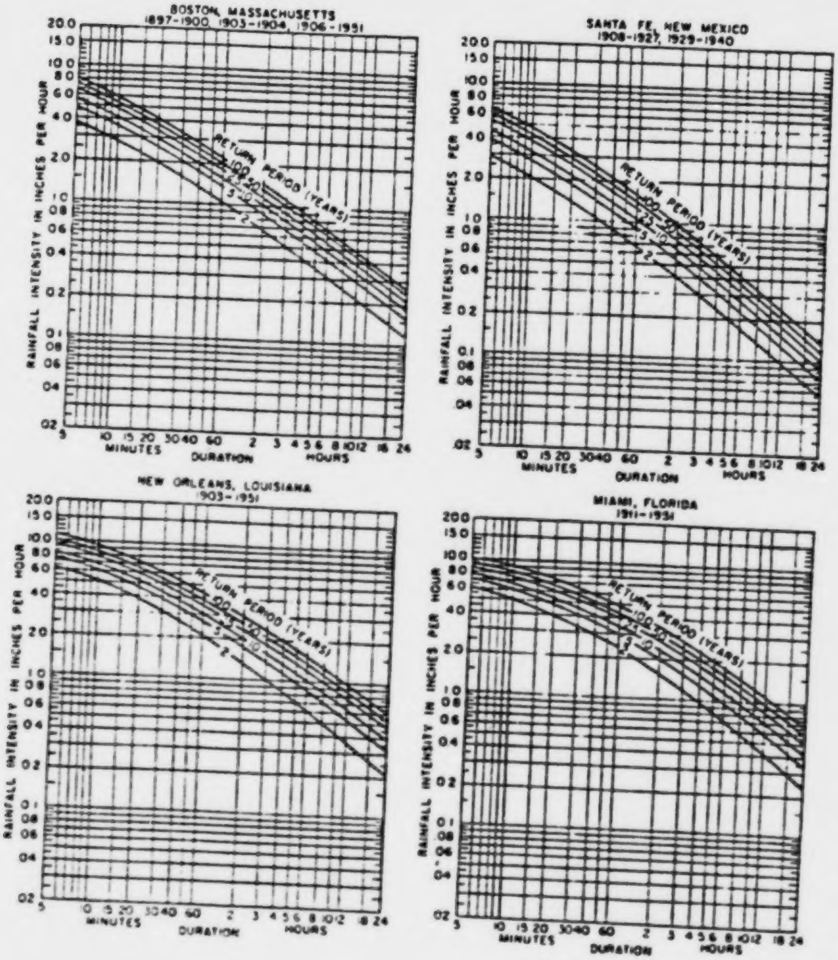
Approaches to Quantity Estimation

The Rational Method[6]

The rational method is perhaps the simplest approach available for estimating runoff volumes and has been employed in various contexts for well over a hundred years (Dooge, 1973). The approach is used to estimate peak flow rates, that is, the maximum rate at which water runs off a catchment during a given precipitation event. Peak flow rates are important for designing stormwater conveyance systems, e.g., sizing storm sewers. The rational method equates peak flow, Q, in cubic feet per second, cfs, to the product of three variables: (1) the area of the catchment, A, in acres; (2) average rainfall intensity, I, in inches/hour, for a given precipitation event; and (3) a runoff coefficient, C_R. Stated in equation form, the relationship is: $Q = C_R \cdot I \cdot A$.[7] The runoff coefficient is always greater than or equal to zero and less than or equal to one ($0 \leq C_R \leq 1.0$). Higher C_R values reflect higher degrees or larger amounts of imperviousness of the land surface in the catchment and smaller losses to evaporation and infiltration. Consequently, high C_R values are typically used for urban areas. Rainfall intensity values are obtained from published intensity-duration-frequency curves, which curves were developed from actual observations. Figure 3-4 illustrates a set of intensity-duration-frequency curves for four U.S. cities. For a complete description of the rational method, see American Society of Civil Engineers and Water Pollution Control Federation (1969). For a critical evaluation of the method, see Schaake, Geyer, and Knapp (1967).

A variant of the rational method is the runoff coefficient method, which involves the same equation but with slightly different runoff coefficients (C_R values). This method is used to predict the average runoff rate over a fixed time period, rather than the peak rate. Prediction of runoff volumes using the runoff coefficient method can be improved by including two additional features: (1) subtraction of depression storage directly from rainfall prior to multiplication by the runoff coefficient; and (2) directly incorporating relationships for predicting the runoff coefficient and amount of depression storage. Runoff coefficients and depression storage are often expressed as functions of land use, soil type, and demographic factors. Applications of modified versions of the runoff coefficient method can be found in Soil Conservation Service (1965); Miller and Viessman (1972); Hydrologic Engineering Center (1977); and Heaney, Huber, and Nix (1976). The crudeness of both forms of the rational method limits their application to situations where only a rough estimate is needed.

Figure 3-4. Intensity-Duration-Frequency Curves for Four U.S. Cities

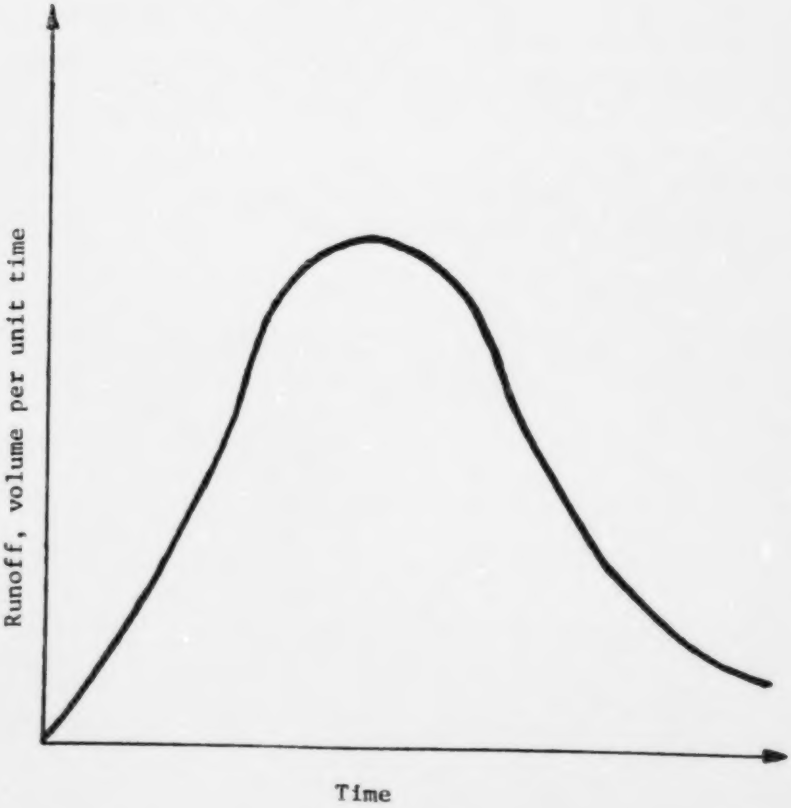


Source: From C. S. Gilman, "Rainfall," in Handbook of Applied Hydrology, Section 9, by V. T. Chow, editor, Copyright 1964 by McGraw-Hill Book Company. Used with permission.

Hydrograph Approach

An hydrograph is a plot of the rate of runoff from a catchment against time for a given storm event, as illustrated in figure 3-5. It may include both direct runoff and base flow. Direct runoff is that portion of rainfall that reaches a designated channel by overland flow or interflow. Base flow is that which occurs between storm events, often due to groundwater inflows, and is not considered part of direct runoff.

Figure 3-5. Hypothetical Hydrograph

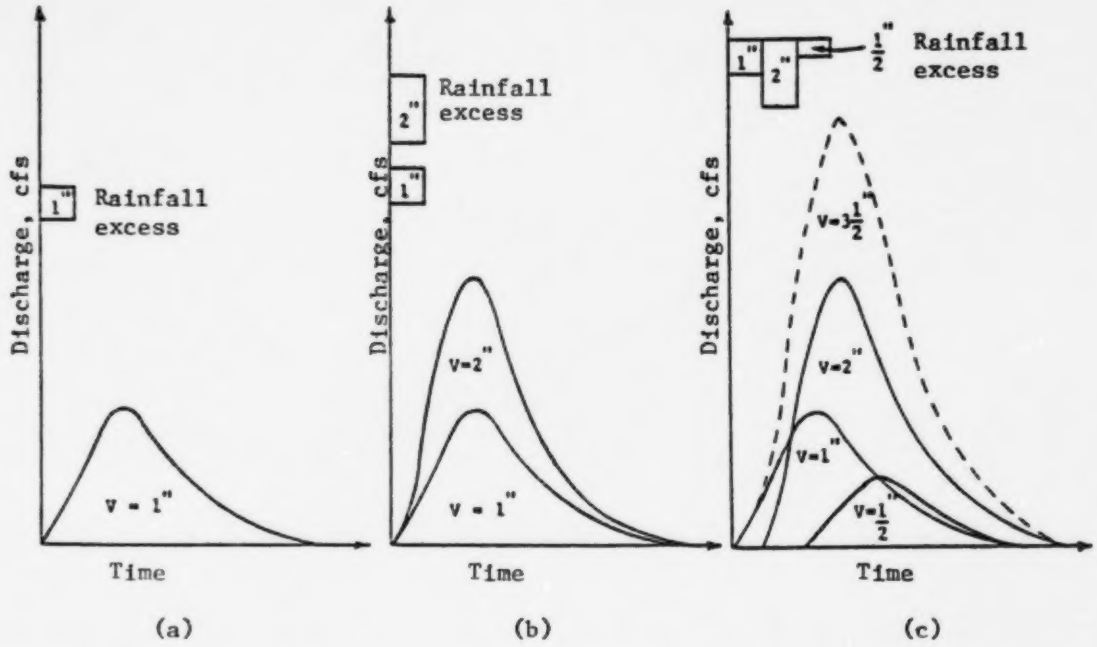


Hydrographs were popularized as an analytical approach for estimating runoff volumes by Sherman (1932) with the development of the unit hydrograph. For a storm of given duration, the unit hydrograph is defined as the hydrograph of direct runoff produced by one inch of rainfall excess--rainfall minus losses--over a catchment. Hydrographs for storms of the same duration but of different intensity, i.e., amount of rainfall or runoff depth, can be obtained from the unit hydrograph by assuming a linear relationship between hydrographs. The procedure is to multiply the ordinates of the unit hydrograph by the actual runoff depth of the storm. This procedure is illustrated in figure 3-6, in which a hypothetical unit hydrograph is given along with examples of direct runoff from a storm producing two inches of rainfall excess, and from a composite storm.

The utility of the hydrograph approach has been greatly increased by the development of methods for generating synthetic unit hydrographs, thereby eliminating the requisite monitoring needed to develop unit hydrographs for individual catchments. One approach for constructing synthetic unit hydrographs is to relate parameters of the unit hydrograph, e.g., peak flow rate, time of peak, flow duration, to catchment properties.[8] Unit hydrographs of this type are derived based on actual flow data and estimates of catchment properties.

Another approach is to assume an analytical form for the unit hydrograph. Unit hydrographs created using this approach are referred to as conceptual hydrographs. It is common to develop conceptual hydrographs based on an instantaneous unit hydrograph. An instantaneous unit hydrograph is the "theoretical" hydrograph which would be produced by an instantaneous rainfall of one inch over a catchment, assuming no losses.[9]

Figure 3-6. Illustration of Unit Hydrograph Procedure



Discharge, cfs
1"
Rainfall excess
V = 1"
Time
(a)
Discharge, cfs
2"
Rainfall excess
1"
V=2"
V = 1"
Time
(b)
Discharge, cfs
1"
2"
1/2"
Rainfall excess
V=3 1/2"
V=2"
V=1"
V=1/2"
Time
(c)

Notes

(a) = Unit hydrograph

(b) = Unit hydrograph applied to storm producing 2 inches of rainfall excess

(c) = Unit hydrograph applied to a composite storm; dashed line is sum of contributions from all three components.

cfs = cubic feet per second

Source: P. E. Morgan and S. M. Johnson, "Analysis of Synthetic Unit-Graph Methods," Journal of the Hydraulics Division, Proceedings of the American Society of Civil Engineers vol. 88, no. HY5 (September 1962) pp. 199-220.

Runoff volumes for storms with arbitrary hyetographs, that is, plots of rainfall intensity versus time, are then computed by linear superposition in a manner analogous to that described above for unit hydrographs (Dooge, 1973).

Because of the extensive use of the instantaneous unit hydrograph, a brief discussion of the derivation of two instantaneous unit hydrograph functional forms--linear reservoir and cascade of linear reservoirs--is warranted. The instantaneous unit hydrograph was dirst derived by recognizing that the instantaneous runoff of one (1) inch of excess rainfall on a catchment is analogous to the discharge from a reservoir whose stored water equals the amount of water represented by the 1 inch of excess rainfall over the catchment area. Opening the gates of the reservoir would be the same as permitting runoff from the catchment to occur instantaneously. Treating an entire catchment as a single reservoir and assuming that outflow is linearly proportional to storage leads to the following equation.

[3-1] $$S = KQ$$

where: S = reservoir storage, ft^3;

Q = reservoir outflow, cfs; and

K = a constant storage coefficient, seconds.

When equation [3-1] is combined with the continuity equation for the reservoir, $I - Q = \frac{dS}{dt}$, where I = inflow to the reservoir, the instantaneous unit hydrograph can be derived (Zoch, 1934, 1936, 1937). The derived exponential form of the instantaneous unit hydrograph for a single linear storage reservoir is:

[3-2] $$IUH(t) = \frac{1}{K} e^{-t/K}$$

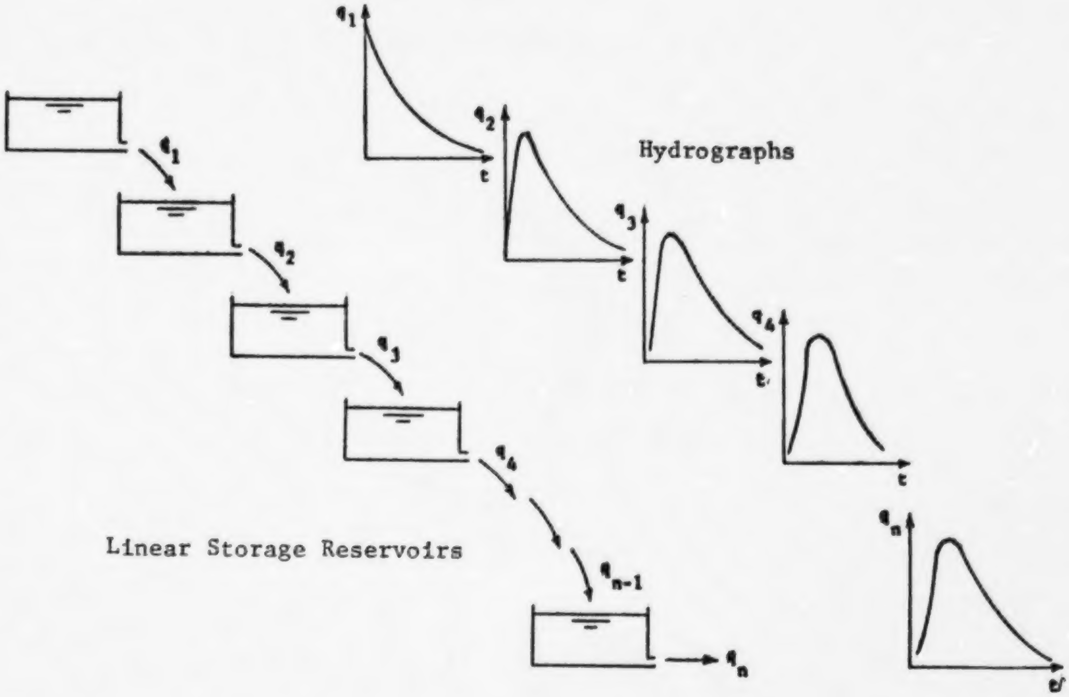
The cascade of linear storage reservoirs form of the instantaneous unit hydrograph is an extension of the single reservoir case and may be conceptualized as a catchment divided into sequential subcatchments for analysis. The procedure involves dividing a river basin into subcatchments according to tributaries, or starting at the head of the river so that each downstream subcatchment empties into the next subcatchment. Each subcatchment is then considered as a separate linear storage reservoir, as illustrated in figure 3-7. Hydrograph q_i, in the upper right portion of the figure, is the exponential instantaneous unit hydrograph for a single linear reservoir, as discussed above. The output from the n^{th} reservoir represents the instantaneous unit hydrograph for the cascade. The following equation was derived by Nash (1957) to represent the instantaneous unit hydrograph for a cascade of n linear reservoirs:

$$[3\text{-}3] \qquad IUH(t) = \frac{1}{K\Gamma(n)}\left(\frac{t}{K}\right)^{n-1} e^{-t/K}$$

where: n = number of equal linear reservoirs, and
$\Gamma(n)$ = gamma function.

The process of summing the responses resulting from a sequence of unit pulses, scaled by the input, e.g., the rainfall hyetograph, is known as convolution and may be performed on discrete or continuous data. For the latter, the convolution integral is also known as the superposition integral or the Duhamel integral (Dooge, 1973). The mathematical problem is to solve the convolution equation for the instantaneous unit hydrograph. For examples see Eagleson, Mejia, and March (1966); Blank and Delluer (1968); Chow and Kulandaiswamy (1971); Amorocho and Brandstetter (1971); and Hossain, Rao, and Delleur (1978).

Figure 3-7. Routing of Instantaneous Inflow Through a Cascade of Linear Storage Reservoirs


q_1
q_2
Hydrographs
q_3
q_4
q_n
t
Linear Storage Reservoirs
q_{n-1}

q = flow

t = time

Source: From V. T. Chow, "Runoff," in Handbook of Applied Hydrology, Section 14, by V. T. Chow, editor. Copyright 1964 by McGraw-Hill Book Company. Used with permission.

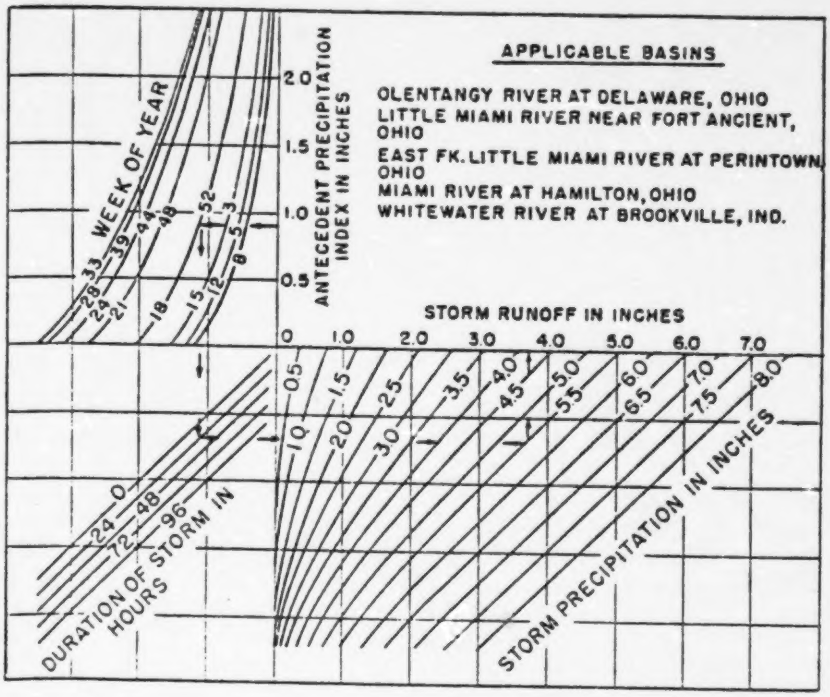
Statistical Approach

The statistical approach for estimating the quantity of water which runs off the land surface is essentially the same as the general statistical approach described in chapter 2. Hence, this section comments only briefly on how the statistical approach has been applied to quantity estimation. In this application the dependent variable is the amount of runoff over a given time interval. Typical independent variables include rainfall, evapotranspiration, soil moisture, antecedent conditions, and base flow.

Prior to the widespread availability of computers and related statistical program packages, various graphic methods were employed to establish relationships between the quantity of runoff and other variables. Some of these methods are still used. Illustrative of these statistically derived "graphical" models are the coaxial relationships derived for several tributary areas of the Ohio River Basin, shown in figure 3-8 (Linsley, Kohler, and Paulhus, 1949). As indicated by the arrows on the figure, the model user would begin with the antecedent conditions and proceed graphically from relationship to relationship to arrive at an estimate of the quantity of runoff. Such graphical models are based on empirical data from specific areas and are not transferable. Of course, the concept of the development of a set of coaxial relationships to estimate runoff is transferable.

Aside from graphical methods, the principal statistical method employed in estimating runoff is regression analysis, although other statistical methods have also had some application.[10] At present it is quite common to use regression analysis results in equation form for estimating runoff volumes (Yevjevich, 1964). Regression methods for analyzing runoff are frequently called API methods because the antecedent precipitation

Figure 3-8. Coaxial Runoff Relations Developed from Data for Several Northern Tributary Areas of the Ohio River Basin



Source: From Applied Hydrology by R. K. Linsley, M. A. Kohler, and J. H. L. Paulhus. Copyright 1949 by the McGraw-Hill Book Company. Used with permission.

index (API) is one of the most used and important independent variables.

An example of a quantity model developed using regression analysis is the following two equation model (Betson, Tucker, and Haller, 1969):

[3-4] $$RI = c + (a + d \cdot SI) \cdot e^{-b \cdot API}$$

[3-5] $$SRO = (RF^n + RI^n)^{1/n} - RN$$

where: SRO = surface runoff from storm even, inches;

RI = runoff index parameter, a function of season;

SI = seasonal index parameter;

API = antecedent precipitation index;

RF = storm precipitation, inches: and

a,b,c,d,n = coefficients of model, determined from data.

This model has been applied in several different watersheds in the Tennessee Valley region. Another example of the use of API methods can be found in Sittner, Schauss, and Monro (1969).

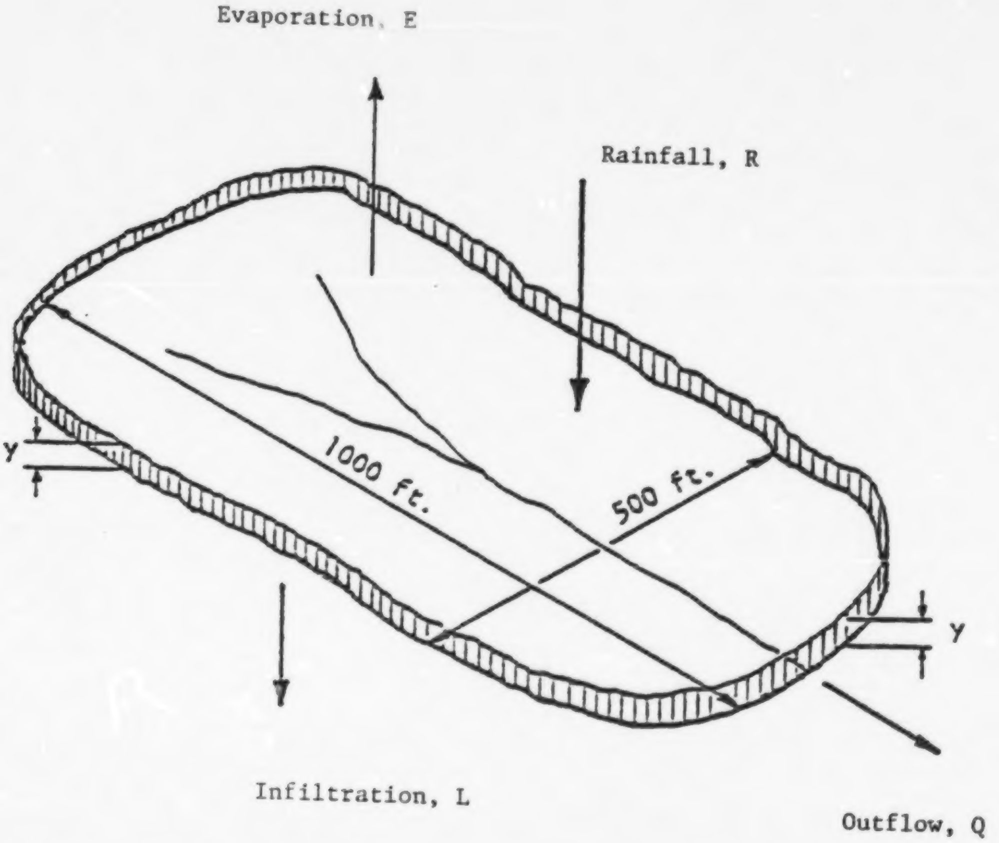
Conservation of Mass and Energy Approach

This approach is based on the fundamental principles of conservation of mass and energy. This discussion assumes familiarity with the section on analytical approaches in chapter 2, in which the fundamentals of the approach and the relevant terminology are described. Regardless of the natural system to which the approach is applied, the fundamentals remain the same.

Central to any application of the conservation of mass and energy approach is the establishment of relevant control volumes. In runoff analysis, a control volume is defined as a hypothetical space above the land surface of a catchment up to a depth of a few feet, as shown in figure 3-9. Depending on the area being analyzed, any number of subcatchments can be defined as control volumes. Figure 3-10 illustrates how a watershed may be divided into subcatchments for analysis. In the actual analysis each subcatchment would be treated as a plane with defined characteristics which affect overland flow, such as slope and surface roughness. Subcatchments are, for purposes of analysis, usually assumed to be connected to other related subcatchments by pipe or channel networks, as illustrated in figure 3-10.

When it rains, the control volume receives inputs, R, and it loses water by infiltration into the ground, L, by surface runoff out of the control volume, Q, and by evaporation, E, as shown in figure 3-9. If R, L, Q,

Figure 3-9. Illustration of a Catchment as a Control Volume

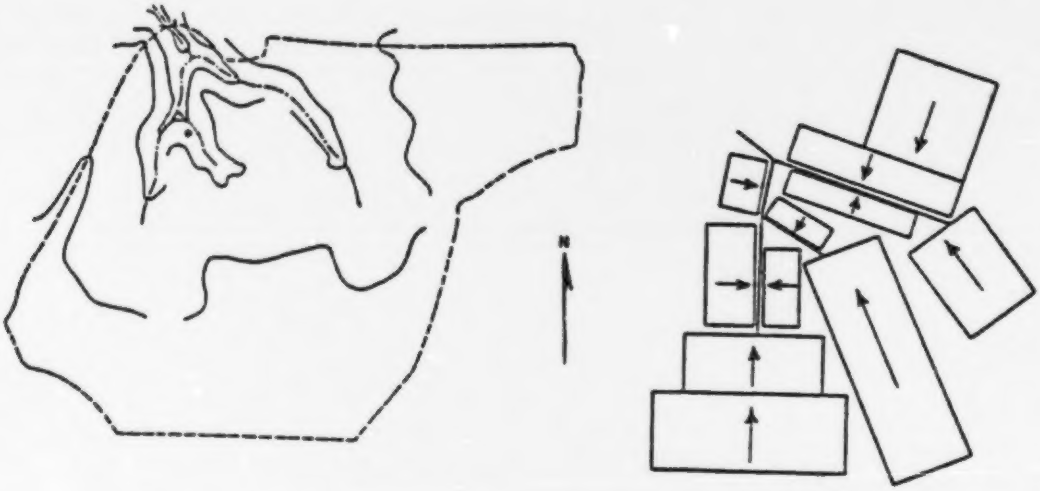


and E represent the amount of water gained or lost by the indicated processes over Δt, then the change in the volume of water, ΔM, in the box can be written as:

[3-6] $$\Delta M = R - L - Q - E$$

Equation [3-6] illustrates the concept of the mass balance principle in relation to the runoff phenomenon. But in order to estimate the rate at which water will run off the land surface, equations which govern the overland flow of water within a control volume must be combined with the mass balance equation. The movement of water--over the land surface, in pipes, in channels, in ditches--is governed by the principle of *conservation of*

Figure 3-10. Illustration of Segmenting a Catchment for Runoff Analysis



Actual Contour Map of Catchment

Schematic Representation of Catchment

Note: Connecting lines represent hypothetical pipes and/or channels connecting subcatchments. Arrows indicate direction of overland flow.

Source: Modified from E. W. Rovey, D. A. Woolhise, and R. E. Smith, A Distributed Kinematic Model of Upland Watersheds, Hydrology Paper 93 (Fort Collins, Colo., Colorado State University, 1977).

momentum. Application of these two principles produces two general equations: the continuity equation and the momentum equation. These equations are typically referred to as the "governing equations" or "equations of motion." In almost all cases, flow is assumed to move in only one direction, e.g., one-dimensional flow.

The governing equations for spatially-varied unsteady flow over a plane were developed by Saint Venant in 1871. But not until the advent of high-speed computers and the development of related numerical estimation methods in the past two decades has it been possible to provide direct solutions for these equations. The governing equations for one-dimensional flow are (Rovey, Woolhiser, and Smith, 1977; Henderson, 1966; and Chow, 1959):

Continuity Equation

$$[3\text{-}7] \qquad \frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} = q$$

Momentum Equation

$$[3\text{-}8] \qquad \frac{1}{g}\left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x}\right] + \frac{\partial h}{\partial x} = S_o - S_f - \frac{q}{g} \cdot \frac{u}{h}$$

where: h = depth of flow;

u = local average velocity;

q = lateral inflow;

x = distance from upstream end;

t = time;

g = acceleration due to gravity;

S_o = slope of the bed surface; and

S_f = the friction slope.

Each term in the momentum equation corresponds to a component of the energy gradient (Rovey, Woolhiser, and Smith, 1977) and hence affects the flow of water. That is:

$\frac{1}{g}\frac{\partial u}{\partial t}$ = the slope due to variation of velocity with time (acceleration);

$\frac{1}{g} u \frac{\partial u}{\partial x}$ = the slope due to variation of velocity with distance in the direction of flow;

$\frac{\partial h}{\partial x}$ = the slope of the water surface; and

$\frac{q}{g} \cdot \frac{u}{h}$ = the slope due to lateral inflow.

The friction slope, S_f, is usually estimated using either the Manning equation or the Chezy equation, as shown below, assuming steady uniform flow at a particular instant and location.

Manning Equation

$$S_f = \frac{u^2 n^2}{1.49^2 R_h^{2/3}}$$

where: u = average velocity, ft/sec;

R_h = hydraulic radius, i.e., the cross-sectional area divided by the wetted perimeter, ft; and

n = Manning roughness coefficient.

Chezy Equation

$$S_f = \frac{u^2}{c^2 R_h}$$

where: c = Chezy roughness coefficient.

For further discussion of the governing equations, see Chow (1959) and Henderson (1966).

The two differential equations shown above comprise the basis for all models for estimating runoff quantity based on the principles of conservation of mass and energy. As described in chapter 2, they can be solved by either analytical or numerical integration methods.[11]

As in all applications of conservation of mass and energy approaches, certain assumptions can be made to simplify application. Two well-known, and extensively used, simplified variations of the equations of motion are the kinematic wave approximation and the lumped continuity formulation.

The kinematic wave approximation to the momentum equation results when it is assumed that the gravity and friction components dominate all other terms in the momentum equation. These two components achieve an approximate equilibrium, thereby reducing the momentum equation to: $S_o = S_f$. Based on this simplified version of the momentum equation, a simple equation for the average velocity results.

$$u = \alpha h^{N-1} \quad [3\text{-}9]$$

where α and N are parameters related to surface roughness. Using Chezy's equation and various algebraic manipulations, both α and N can be determined. Therefore, combining equation [3-9] with the continuity equation, [3-7], yields a solvable set of two equations and two unknowns--u (velocity) and h (depth).[12] However, in spite of the relative simplicity of the kinematic wave formulation compared to the Saint Venant equations, numerical integration methods are still required to solve most kinematic wave formulations.

Kinematic wave formulations have been shown to be particularly applicable for estimating overland flows (Eagleson, 1970) and often for estimating channel flow as well. These formulations are typically used to analyze individual runoff events and have been found to produce satisfactory results for both urban and agricultural areas. Numerous references are available in the literature.[13]

The lumped continuity formulation uses the continuity equation in a very aggregated, i.e., "lumped," form by simply equating a change in volume, with no spatial variation, to the sum of inflows minus outflows. Thus, $\frac{dS}{dt} = I - Q$, where S = volume, I = inflow, and Q = outflow. This formulation is analogous to the simple mass balance equation presented earlier as equation [3-6]. If the outflow is assumed to be linearly proportional to storage volume, the previously described linear reservoir results. If a nonlinear relationship is used a nonlinear reservoir results.

In summary, most models for estimating runoff quantity attempt to include as many aspects of the hydrologic cycle as possible in their formulations. This almost invariably leads to a combination of approaches in which different methods are applied to different components of the rainfall-runoff cycle. For example, unit hydrographs or kinematic waves may be used to generate overland flow; "storage reservoirs" in various series-parallel combinations may be used to simulate subsurface flow; and kinematic waves or the complete Saint Venant equations may be used for channel flow routing.[14] The large number of models presently available to estimate runoff quantity is a direct result of the number of approaches available for analyzing various parts of the hydrographic cycle and of the ways in which they can be combined.

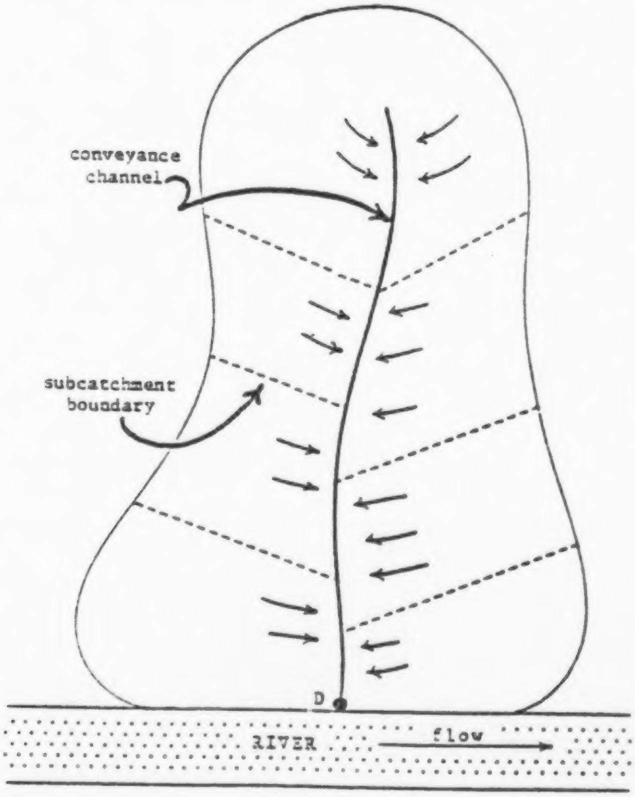
Approaches to Quality Estimation

Three introductory comments to the discussion of quality estimation are in order. First, although there are many residuals which are carried off the land surface by runoff, until recently only one of these residuals, sediment, received much attention. This is because of early recognition of the costly effects of soil erosion on soil productivity and of sediment deposition in reservoirs, as mentioned earlier. Consequently, there is a relative abundance of approaches, experience, and related literature on estimating sediment discharges due to runoff compared to estimating discharges of other residuals due to runoff.[15] This is true for both urban and nonurban areas. Besides sediment, typical residuals in runoff include nitrogen, phosphorus, chemicals such as pesticieds and phenols, lead, oil and grease, organic materials, and heavy metals.

Second, NSMs based on conservation of mass and energy principles are seldom, if ever, used to estimate the quality of runoff from land surfaces. Typically, such NSMs are used to route residuals in runoff waters only after they have entered conveyance channels. The application of conservation of mass and energy principles in conveyance channels is analogous to their application to streams and rivers, i.e., the transport block, as described in chapter 4.

Third, given the situation depicted in figure 3-11, there are two procedures for estimating the quantities of residuals discharged from a given land area to a receiving water body. One is to estimate the quantities of residuals generated in each subcatchment that reach the conveyance

Figure 3-11. Representation of a Catchment Area for Estimating Residuals Discharges to a Receiving Water Body



channel using a statistical model; then to route the residuals in the conveyance channel to the discharge point to the river, D, using a conservation of mass and energy model. The other is to estimate the quantities of residuals entering the river at point D from the entire catchment using only a statistical model.

Statistical Approach

Models for estimating runoff quality based on the statistical approach are of two general types. The first utilizes a statistical technique, most often regression analysis,[16] to produce a statistical relationship between quality, i.e., quantity or concentration of a residual, and relevant independent variables. Because the principles for applying regression analysis are universal and are discussed in chapter 2, no further discussion of this type is included here.

The second type involves positing a functional relationship between quality and relevant variables based on knowledge of the physical processes involved, e.g., that soil erodibility will affect the quantity of soil eroded. Values for each of the posited variables are developed for different sets of conditions, from empirical measurements on experimental plots or under actual field conditions. The most well-known and widely used statistical model of this second type is the Universal Soil Loss Equation (USLE), used to estimate gross sediment discharge from a land surface. The USLE is:

$$M = R \cdot K \cdot LS \cdot C \cdot P \qquad [3\text{-}10]$$

where: M = soil loss from rainstorms, ton/acre/time period;

R = rainfall factor/time period;

K = soil erodibility factor;

LS = slope-length, slope-gradient factor;

C = crop management factor or cover index factor; and

P = erosion control practice factor.

The rainfall factor reflects the fact that soil erosion has been found, in the eastern United States, to be directly proportional to the product of the kinetic energy of a storm and the maximum thirty-minute intensity of the storm. This product is characterized as the erosion index. To estimate mean annual soil loss from a given land area, the rainfall factor, R, equals the total number of erosion index units associated with the mean distribution of rainfall events in a year. The soil loss in a year from any other distribution of rainfall events can of course also be estimated. Suggested annual values of the erosion index to use for various parts of the United States have been developed and are available in maps and charts, as in Stewart, et al. (1975). The following equation, developed from data from many storms, can be used to estimate the rainfall factor, R, to be used in equation [5-4].

$$R = I \cdot \sum_{j=1}^{n} (9.16 + 3.31 \log_{10} i_j)d_j \qquad [3\text{-}11]$$

where: I = maximum average 30-minute rainfall intensity, in/hr;

i_j = rainfall intensity during time interval j, in/hr;

d_j = depth of rainfall during time interval j, in.; and

n = number of time intervals during the rainfall event.

The values of the otehr factors in the USLE, e.g., K, LS, C, and P, have likewise been developed from experimental and field data. The data are typically tabulated in tables and graphs, such as in SCSA (1977) and EPA (1973) for K; Griffin (1975) and SCS (1975a) for C; and True (1974) for P. Empirical formulae to calculate LS values have been developed, such as the following (SCS, 1975a).

[3-12] $$LS = \left(\frac{\lambda}{72.6}\right)^m \left(\frac{430x^2 + 30x + 0.43}{6.57415}\right)$$

where: λ = field slope length, ft.;

m = 0.5 if slope equals 5% or greater,

= 0.4 if slope equals 4%,

= 0.3 if slope equals 3% or less; and

x = sine of the slope angle.

The USLE was developed primarily for estimating soil loss from agricultural cropland in temperate climates. However, many modified forms of the equation have been developed to enable making estimates of sediment in runoff for land uses other than agricultural cropland. Numerous references are available describing every aspect of applying the USLE, for example Wischmeier and Smith (1965), EPA (1973), and McElroy, et al. (1976). However, the equation is not directly applicable for estimating soil erosion from snowmelt or from the application of irrigation water.[17]

It is important to emphasize that the USLE does not estimate the amount of sediment which actually enters a receiving water body, but rather estimates the "gross" amount of soil (sediment) which erodes from a given land area up to the edge of that land area. To estimate how much of the gross eroded soil enters a receiving water body, the gross amount of soil eroded muxt be multiplied by a factor, the sediment delivery ratio. Sediment delivery ratios are approximations, and have been estimated from field observations.

The USLE can also be used to estimate the quantities of other residuals washed off the land surface to the extent that other residuals can be directly related to sediment runoff. An example is the following equation (McElroy, et al., 1976) for estimating nitrogen in runoff from agricultural cropland:

[3-13] $$NT_E = 20 \cdot M \cdot A \cdot (NT)_s \cdot r_N$$

where: NT_E = total nitrogen load from soil erosion, lb/yr;

M = average annual soil erosion estimated by equation [3-10], ton/acre/yr;

A = land surface area, acres;

$(NT)_s$ = total nitrogen concentration in soil, g/100g (i.e., percent by weight); and

r_N = nitrogen enrichment ratio, i.e., the nitrogen content of the eroded soil divided by $(NT)_s$.

The coefficient, 20, was determined empirically from a number of observations; the values of $(NT)_s$ and r_N are measured for each case. To estimate how much of the estimated nitrogen load actually enters a receiving water body, a sediment delivery ratio would have to be applied to the total nitrogen load estimated by equation [3-13].

Another example of the second type of statistical model for estimating quality is the exponential washoff function. In this model, the rate at which a residual washes off a land area is assumed to be proportional to the amount of the residual on that surface available for washoff. Coefficients for the model are determined on the basis of measured residuals concentrations in runoff. The equation for the exponential washoff function is:

[3-14] $$P = P(t) \cdot e^{-\beta \cdot r \cdot \Delta t}$$

where: P = mass of residual remaining on the surface at the end of time step Δt, lb;

$P(t)$ = mass of residual on surface at beginning of time step Δt, lb;

β = empirical coefficient, in^{-1};

r = runoff (flow) rate, in/hr; and

Δt = time step, hr.

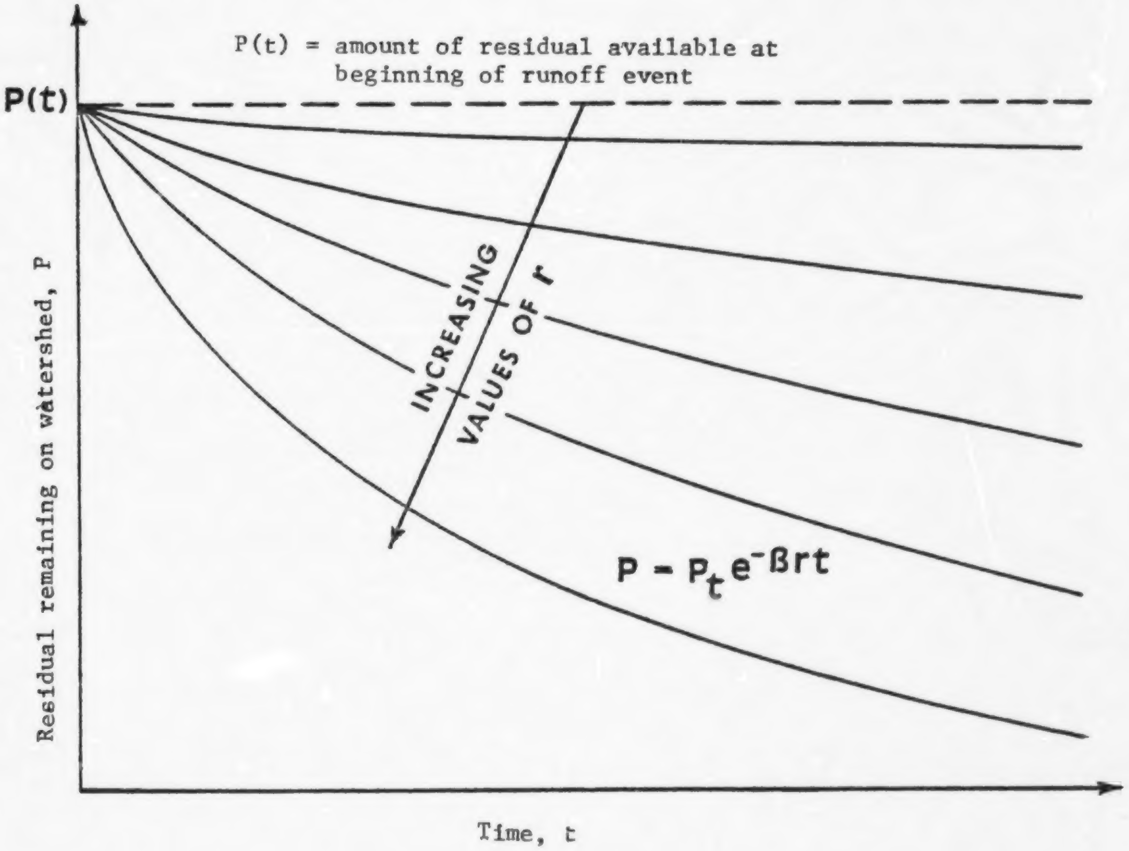
The coefficient, β, is selected based on an assumption about the rate at which residuals are removed from the land surface. For example, a frequently used--but unverified--assumption is that a runoff rate of 0.5 in/hr will remove 90 percent of the mass of a residual on the land surface in one hour, resulting in a β value of 4.6 in^{-1}. If an initial quantity, $P(t)$, is assumed available at the beginning of a runoff event, equation [3-14] can be rewritten and graphed as shown in figure 3-12. Note that the washoff rate increases as r increases. Washoff functions have been used extensively in analyses of urban areas and, in spite of their limitations, have produced reasonable results when adequately calibrated.

Numerous other equations have been developed to estimate quantities of various residuals washed off the surface of a given land area. For example, see AVCO Economic Systems Corporation (1970); Sartor and Boyd (1972); Colston (1974); Hammer (1976); McElroy, et al. (1976); and Heaney, Huber and Nix (1976). However, those presented herein are indicative of the general statistical approach taken when a functional form is posited and are the most frequently used approaches to date.

Conservation of Mass and Energy Approach to Quality Estimation

As indicated previously, the use of the conservation of mass and energy approach is restricted, in the context of estimating runoff quality,

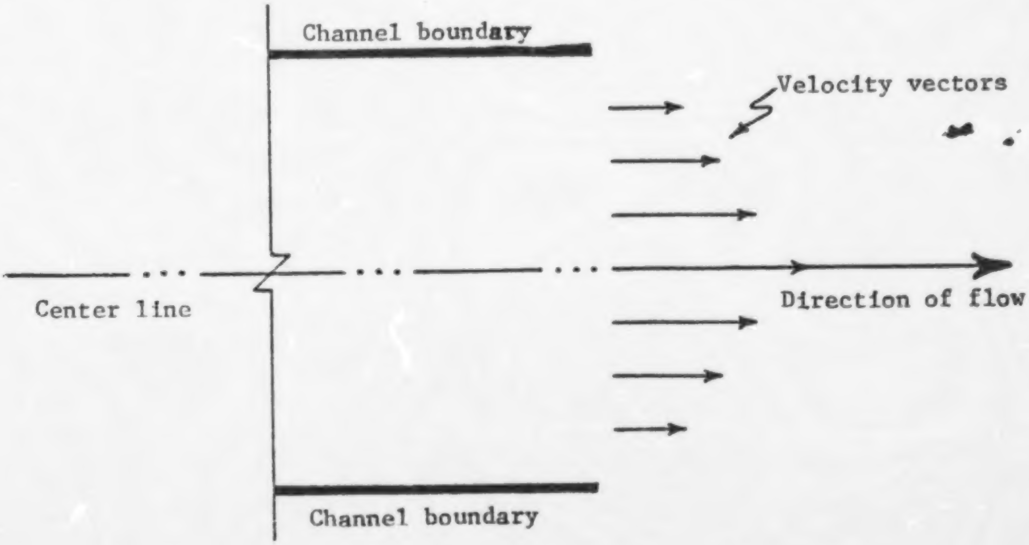
Figure 3-12. Illustration of Exponential Washoff Function with Varying r Values



Source: L. A. Roesner, H. M. Nichandros, R. P. Shubinski, A. D. Feldman, J. W. Abbott, and A. O. Friedland, A Model for Evaluating Runoff-Quality in Metropolitan Master Planning, Technical Memo No. 23 (New York, American Society of Civil Engineers Urban Water Resources Research Program, 1974); also available as NTIS Publication No. PB-234-312.

to estimating temporal and spatial patterns of residuals concentrations after the runoff has entered a conveyance channel. Because this application is analogous to the application of these principles to receiving water bodies, as described in chapter 4, little additional discussion is necessary here. However, a few points merit comment. First, in almost all cases of application to conveyance channels, only a one-dimensional analysis is employed where velocities and residuals concentrations represent cross-sectional averages and all variation within a channel cross-section is averaged out. The distribution of these spatially averaged concentrations reflects velocity variations between the channel bottom and sides (zero velocity) and the channel center (maximum velocity), as shown in figure 3-13. The effect of velocity variations is to increase longitudinal spreading of residuals and may be treated as an additional diffusion mechanism, i.e., longitudinal dispersion, in the conservation of mass and energy equations (Holley, 1969).

Figure 3-13. Illustration of Distribution of Velocity in Channelized Flow



Second, residuals transport in conveyance channels is most often simulated as a purely advective process, or else as a linear series of completely mixed channel sections. The former is probably more realistic, because diffusion has little impact on residuals concentrations relative to advection in rapidly flowing water (Dobbins, 1964).

Third, because of the rapid rate of flow in conveyance channels and subsequent short travel times to receiving water bodies, especially in urban areas, chemical reactions and ecological processes are not typically considered.

Summary Comments on Quantity/Quality Estimation

In order to estimate both the quantity and quality of runoff waters in one computational framework, some combination of the analytical approaches for each aspect is necessary. Whatever the combination, explicit consideration of antecedent precipitation events, and hence of antecedent soil moisture conditions in pervious areas, is likely to be important.

Different combinations of approaches are employed in the various quantity/quality runoff models that have been developed to date. The combination of approaches chosen in any given model is a function of the characteristics of the runoff problem or problems the model is designed to address. Characteristics of runoff problems which affect the analytical approaches chosen include: type of land area; temporal properties; spatial properties; relevant hydrologic and hydraulic processes to be considered; and relevant physical, physicochemical, and biochemical processes in relation to the residuals of interest.

SELECTING AN APPROPRIATE RUNOFF MODEL

This section has two purposes. The first is to assist an analyst in the determination of whether or not the runoff analysis specified to answer questions posited is feasible to carry out, given the conditions specified for the REQM analysis. The second is to assist in the selection of an NSM for application based on other relevant criteria.

The section corresponds to the section on setting up the natural systems analysis in chapter 2, which indicated that there is a logical sequence of steps to follow to determine what type of natural systems analysis to undertake in any given context. Six steps were identified and described in table 2-3. The fourth step in the sequence is related to determining the feasibility of carrying out the natural systems analysis specified in the previous three steps. The fifth step is related to selecting an NSM for application based on relevant evaluation criteria. The material in this section is therefore an extension of these two steps, given a context in which analysis of residuals discharges from the land surface is required.

Five elements comprise the section: (1) a listing of a large number of runoff models, both operational and nonoperational--the population table; (2) a table which relates characteristics of runoff problems to the operational NSMs in the population table--the problem table; (3) a flow diagram which indicates how to select an appropriate runoff model using the material included in the chapter--the selection procedure; (4) a discussion of the model characteristics which are used to summarize each of the operational runoff models; and (5) summaries of the characteristics of the operational runoff models--the model summary tables. Model summary tables for fourteen runoff models are contained in Appendix A to the chapter.

Population of Runoff Models

Table 3-1 lists the runoff models which were reviewed in preparation of this chapter. This compilation does not represent the total set of developed runoff models. Literally hundreds of models have been developed over the years, including many models which do not involve the use of a computer and are often simply referred to as analytical procedures. Models have been documented in the form of reports, journal and proceedings articles, texts, and personal communications. The seventy-three listed in table 3-1 are models that are known to have been applied to actual problems. Most of the models listed have been developed using "public" funds, developed either directly by a public agency or by a university or consulting firm supported by a public agency. Consequently, most of the models listed could be obtained and used by others. However, this does not mean that the documentation available for most models is good enough to permit application without considerable effort. In fact, available documentation is seldom adequate.

The models in the table have been grouped into four categories based on level of complexity: (1) screening procedures; (2) simplified computer models; (3) continuous simulation models; and (4) single event simulation models.[18] Within the category of continuous simulation models, there are two subcategories, Stanford Watershed Model variants and other models. The table also indicates: the general type of land area to which a model is applicable, urban or nonurban; whether or not a model analyzes the quality aspect of runoff; and the relative experience with the model in relation to application. References are provided in the table for runoff models which are not summarized in Appendix A.

Table 3-1. Population of Runoff Models

Name	Commonly Used Acronym	Originator	Applicable Land Area	Level	Quality	Experience with Model[a]	References
Screening Procedures							
Hydroscience Simplified Model	---	Hydroscience, Inc., Westwood, N.J.	Urban	I	Yes	C	*[b]
Storm Water Management Model, Level I	SWMM-Level I	Dept. of Environmental Engineering Sciences, Univ. of Florida, Gainesville, Fla.	Urban	I	Yes	C	*
Midwest Research Institute Loading Functions	MRI	Midwest Research Institute, Kansas City, Mo.	Nonurban,[c] Urban	I	Yes	C	*
Rainfall-Runoff Relations on Urban and Rural Areas	---	Univ. of Michigan, Ann Arbor, Mi.	Urban, Nonurban	I	None	A	Brater and Sherrill, 1975
Theory of Storage and Treatment Plant Overflows	---	C.D.D. Howard Associates, Winnipeg, Manitoba	Urban	I	None	B	Howard, 1976
Water Quality Management Planning for Urban Runoff	---	URS Research Co San Mateo, Ca.	Urban	I	Yes	B	Amy, et al. (1974)
Simplified Computer							
Rational Method	---	---	Urban	I,II	None	C	American Society of Civil Engineers and water Pollution Control Federation, 1969, Schaake, Geyer and Knapp, 1967,
Los Angeles Hydrograph Method	---	City of Los Angeles Los Angeles, Ca.	Urban	I,II,	None	C	Hicks, 1944
Santa Barbara Urban Hydrograph Method	SBUH	Santa Barbara County Flood Control and Water Conservation District, Santa Barbara, Ca	Urban	II	None	B	Stubchaer, 1975
Environmental Pollution Assessment-Erosion, Sedimentation and Rural Runoff Model	EPARRB	National Environmental Research Center, Environmental Protection Agency, Athens, Ga.	Nonurban	II	Yes	B	*
Huggins and Monke	---	Department of Agricultural Engineering, Purdue Univ., Lafayette, In.	Nonurban	II	None	A	Huggins and Monke, 1966
Semi-Arid Catchment Model	---	Univ. of Arizona, Tucson, Az.	Nonurban	II	None	A	Fogel and Duckstein, 1970 Arai, et al., 1975
TVA Stormwater Model	---	Div. of Water Control Planning, Tennessee Valley Authority, Knoxville, Tn.	Nonurban	II	None	B	Ardis, 1973

Table 3-1. Population of Runoff Models (Continued)

Name	Commonly Used Acronym	Originator	Applicable Land Area	Level	Quality	Experience with Model ^a	References
Simplified Computer							
Management of Urban Nonpoint Pollution	MUNP	Dept. of Civil Engineering Univ. of Maryland, College College Park, Md.	Urban	II	Yes	A	Sutherland and McCuen, 1978
Simplified Storm Water Management Model	Simplified SWMM	Metcalf and Eddy, Inc. Palo Alto, Ca.	Urban	II	Yes	B	*
Continuous Simulation							
a. Stanford Watershed Model Variants							
Stanford Watershed Model IV	SWM-IV	Department of Civil Engineering, Stanford Univ., Palo Alto, Ca.	Nonurban	III	None	C	Crawford and Linsley, 1966
Texas Watershed Model	TWM	Univ. of Texas, Austin, Tx.	Nonurban	III	None	A	Claborn and Moore, 1970
Kentucky Watershed Model	KWM	Univ. of Kentucky, Lexington, Ky	Nonurban	III	None	C	James, 1970, Liou, 1970 Ross, 1970
Self-Optimizing, Continuous Hydrologic Simulation Model	OPSET	Univ. of Kentucky, Lexington, Ky	Nonurban	III	None	C	" "
Ohio State University Version of SWM-IV	OSUSWM	Ohio State Univ., Columbus, Oh.	Nonurban	III	None	A	Ricca and Warns, 1972
Georgia Tech Watershed Simulator	GTWS	Dept. of Civil Engineering, Georgia Tech Univ., Atlanta, Ga	Nonurban	III	None	B	Lumb, et al., 1975
National Weather Service River Forecast System	NWSRFS	Office of Hydrology, National Weather Service, Silver Spring, Md.	Nonurban	III	None	B	National Weather Service, 1972
Sacramento Model	---	National Weather Service River Forecast Center and State of California Dept. of Water Resources, Sacramento, Ca.	Nonurban	III	None	B	Burnash, Ferral and McGuire, 1973
TVA Daily Flow Model	TVA	Div. of Water Control Planning, Tennessee Valley Authority, Knoxville, Tn.	Nonurban	III	None	B	Betson, 1972
Digital Hydrologic Simulation Model	---	Clemson Univ., Clemson, Sc.	Nonurban	III	None	A	Ligon, Law and Higgons, 1969
Hydrocomp Simulation Program	HSP	Hydrocomp, Inc. Palo Alto, Ca.	Nonurban, Urban	III, IV	Yes	C	*
Pesticide Transport and Runoff Model	PTR	Hydrocomp, Inc., Palo Alto, Ca.	Nonurban	III	Pesticides	B	Crawford and Donigian, 1973
Agricultural Runoff Management Model	ARM	Hydrocomp, Inc., Palo Alto, Ca.	Nonurban	III, IV	Yes	C	*
Nonpoint Source Model	NPS	Hydrocomp, Inc., Palo Alto, Ca.	Nonurban	III	Yes	C	*

Table 3-1. Population of Runoff Models (Continued)

Name	Commonly Used Acronym	Originator	Applicable Land Area	Level	Quality	Experience with Model [a]	References
Continuous Simulation							
Terrestrial Ecosystem Hydrology Model	TEHM	Oak Ridge National Laboratory, Oak Ridge, Tn.	Nonurban	III	Yes	B	Patterson, et al., 1974
Other Continuous Simulation Models							
Simulation of Contaminant Reactions and Movement	SCRAM	ESL Inc., Sunnvale, Ca.	Nonurban	III	Yes	B	Adams and Kurisu, 1976
Agricultural Chemical Transport Model	ACTMO	Agricultural Research Service, USDA, Beltsville, Md.	Nonurban	III	Yes	C	*
Numerical Model for Runoff and Sediment Discharge Estimation	---	Dept. of Civil Engineering at Univ. of Waterloo, Waterloo, ON and McGill Univ., Montreal, PQ	Nonurban	III	Sediment	A	Solomon and Gupta, 1977
Streamflow Synthesis and Reservoir Regulation	SSARR	North Pacific Div., Corps of Engineers, Portland, Or.	Nonurban	III	None	C	U.S. Army Corps of Engineers, 1972 Rockwood, Davis and Anderson, 1972
Conversational Streamflow Synthesis and Reservoir Regulation Program	COSSARR	" "	Nonurban	III	None	B	Rockwood, Davis and Anderson 1972
Storage, Treatment, Overflow and Runoff Model	STORM	Hydrologic Engineering Center, Corps of Engineers, Davis, Ca.	Urban Nonurban	III	Yes	C	*
Southeast Michigan Council of Governments Storage, Treatment, Overflow and Runoff Model	SEM-STORM	Water Resources Engineers, Inc., Springfield, Va.	Urban	III	Yes	A	Shubinski, Knepp and Bristol, 1977a, 1977b
Quantity-Quality-Simulation Model	QQS	Dorsch Consult, Munich, Germany and Toronto, ON	Urban	III, IV	Yes	C	*
MIT Catchment Model	MITCAT	Dept. of Civil Engineering, Mass Institute of Technology, Cambridge, Ma. and Resource Analysis Inc., Waltham, Ma.	Nonurban Urban	III, IV	Sediment	C	Resource Analysis Inc., 1975 Harley, Perkins and Eagleson, 1970
Single Event Simulation							
U.S. Dept. of Agriculture Hydrological Laboratory Model	USDAHL-74	Agricultural Research Service, USDA, Beltsville, Md.	Nonurban	IV	None	C	Holtan, et al., 1975
Problem Oriented Computer Language for Hydrologic Modeling	HYMO	Agricultural Research Service, USDA, Soil and Water Conservation Research Div., Riesel, Tx.	Nonurban	IV	None	B	Williams and Hann, 1972, 1973
Computer Program for Project Formulation Hydrology	TR-20	C-E-I-R, Inc., for Soil Conservation Service, USDA, Washing- Washington, D.C.	Nonurban	IV	None	C	Soil Conservation Service, 1965

Table 3-1. Population of Runoff Models (Continued)

Name	Commonly Used Acronym	Originator	Applicable Land Area	Level	Quality	Experience with Model a	References
Single Event Simulation							
Urban Hydrology for Small Watersheds	TR-55	Soil Conservation Service, USDA, Washington, D.C.	Urban	I, II, IV	None	C	Soil Conservation Service, 1975b
Water-Sediment-Chemical Watershed Runoff Model	WASCH	Agricultural Research Service, USDA, Athens, Ga.	Nonurban	IV	Pesticides	A	Bruce, et al., 1973
OKI Rural Runoff Model	OKI-RRM	Ohio-Kentucky-Indian Council of Governments, Cincinnati, Oh.	Nonurban	IV	Yes	A	Ohio-Kentucky-Indiana Reg. Council of Govts., 1975
Agricultural Runoff Model	AGRUN	Water Resources Engineers, Inc., Walnut Creek, Ca.	Nonurban	IV	Yes	C	*
U.S. Geological Survey Rainfall Runoff Model for Peak Flow Synthesis	USGS	U.S. Geological Survey, Reston, Va.	Nonurban Urban	IV	None	C	Dawdy, Lichty & Bergman, 1972 Dawdy and O'Donnell, 1965
Kinematic Wave Generation Model	KINGEN	Agricultural Research Service, USDA and Colorado State Univ., Fort Collins, Co.	Nonurban Urban	IV	None	A	Woolhiser, 1977b Rovey and Woolhiser, 1977
Battelle Urban Wastewater Management Model	BNW	Battelle Pacific Northwest Lab., Richland, Wa.	Urban	IV	Yes	B	Brandstetter, Engel and Cearlock, 1973 Brandstetter, 1976
Calcul des Reseaux D'assainissement (Calculation of Sewage Networks)	CAREDAS	SOGREAH, Grenoble, France (also New York, N.Y.)	Urban	IV	Yes	C	*
Computer Augmented Treatment and Disposal System	CATAD	Municipality at Metropolitan Seattle, Seattle, Wa.	Urban	IV	None	A	Leiser, 1974
Chicago Hydrograph Method	CHM (also NERO)	City of Chicago Bureau of Engineering, Chicago, Ill.	Urban	IV	None	C	Tholin and Keifer, 1959 Keifer, Harrison and Hixson, 1970
Chicago Flow Simulation Programm	FSP	Metropolitan Sanitary District of Greater Chicago, Chicago, Ill.	Urban	IV	None	B	Lanyon and Jackson, 1974a, 1974b
City of Chicago Runoff Simulation Model	---	City of Chicago Dept. of Public Works, Chicago, Ill.	Urban	IV	Yes	A	City of Chicago, 1972
Dynamic Model for Urban Hydrologic Systems	HYDRA	Dept. of Computer Science, Univ. of Nebraska, Lincoln, Nb.	Urban Nonurban	IV	None	A	Surkan, 1973, 1974 Surkan and Kelton, 1974
HEC-1 Flood Hydrograph Package	HEC-1	Hydrologic Engineering Center, Corps of Engineers, Davis, Ca.	Nonurban	IV	None	C	Hydrologic Engineering Center 1973
Hydrograph Volume Method	HVM	Dorsch Consult Munich, Germany (also Toronto, On.)	Urban	IV	None	C	Klym et al., 1972 Dorsh Consult Ltd., 1974
Illinois Storm Sewer System Simulation Model	ISS	Dept. of Civil Engineering, Univ. of Illinois, Urbana, Ill.	Urban	IV	Preliminary	B	Sevuk, Yen and Peterson, 1973

Table 3-1. Population of Runoff Models (Continued)

Name	Commonly Used Acronym	Originator	Applicable Land Area	Level	Quality	Experience with Model *	References
Single Event Simulation							
Illinois Surface Runoff Model	ISRM	Dept. of Civil Engineering, Univ. of Illinois Urbana Ill.	Urban	IV	Preliminary	B	Chow and Yen, 1976
Illinois Urban Drainage Area Simulator	ILLUDAS	Illinois State Water Survey Urbana Ill.	Urban	IV	Preliminary	C	Terstreip and Stall, 1974
Norwegian Institute of Water Research Model	NIVA	Norwegian Institute of Water Research Blindern, Norway	Urban	IV	Yes	B	Lindholm, 1976
Penn State Urban Runoff Model	PSURM	Dept. of Civil Engineering, The Pennsylvania State Univ., University Park, Pa.	Urban	IV	None	B	Aron and Lakatos, 1976
Queen's University Urban Runoff Model	QUURM	Dept. of Civil Engineering, Queen's Univ., Kingston, On.	Urban	IV	None	A	Watt and Kidd, 1975
Road Research Laboratory Model	RRL	Transport and Road Research Laboratory, London, United Kingdom	Urban	IV	None	C	Watkins, 1963 Terstrein and Stall, 1969 Stall and Terstrein, 1972
Storm Runoff-Quality Model	RUNQUAL	Water Resources Engineers, Inc. Walnut Creek, Ca.	Urban	IV	Yes	A	Roesner, Giguere & Davis, 1977 Roesner and Giguere, 1977
Storm Water Management Model	SWMM	Metcalf and Eddy, Palo Alto Ca; Univ. of Florida, Gainesville, Fla; Water Resources Engineers, Walnut Creek Ca.	Urban Nonurban	III, IV	Yes	C	*
Texas A & M Model	QUANT-QUAL	Dept. of Civil Engineering, Texas A & M Univ., College Station, Tx.	Urban	IV	Yes	A	Malouf, 1974
Texas Tech Model	---	Texas Tech Univ., Water Resource Resources Center, Lubbock, Tx.	Urban	IV	Yes	A	Wells, Austin and Cook, 1971
University of Cincinnati Urban Runoff Model	UCUR	Dept. of Civil Engineering, Univ. of Cincinnati, Cincinnati, Oh.	Urban	IV	None	C	Preul and Papadakis, 1970 Papadakis and Preul, 1972
University of Massachusetts Combined Sewer Control Simulation Model	HYDROL	Dept. of Civil Engineering, Univ. of Mass., Amherst, Ma.	Urban	IV	None	A	Ray, 1973
Urban Runoff Model PDP-9	URCM-9	St. Anthony Falls Hydraulic Lab. Univ. of Minnesota, Minneapolis Mn.	Urban	IV	None	B	Harris, 1970 Pabst, Bowers&Harris, 1971
Wastewater Collection System Model	SAM	CH2M-Hill, Inc., Corvallis, Or.	Urban	IV	None	B	O'Neel, Davis & Vandusen, 1976
Wilsey and Ham Model	WH-1	Wilsey and Ham Consulting Engineers, Foster City, Ca.	Urban	IV	None	A	Amorocho, 1972

Table 3-1. Population of Runoff Models (Continued)

Note: [a]Categories of experience with model are:

A. Use of model or analytical procedure limited primarily to model developer; few or no references to application and testing by others;

B. Some use of model or analytical procedure by others or extensive use by model developer; and

C. Extensive, continued use of model or analytical procedure by model developer and others.

[b]Asterisk (*) indicates model is included in summary tables. References are listed in Appendix B for each such model. All other references are given in general list of references.

[c]When both urban and nonurban land areas are given, the first listed represents the primary or original orientation of the model or analytical procedure.

From the compilation of models listed in table 3-1, detailed summaries were made of fourteen operational models. These models are identified with an asterisk in the last column of the table. Note that in addition to the fourteen models summarized, other models in table 3-1 are also operational. These other operational models have not been summarized because they are very similar to, or are variations of, one of the models which is summarized. To reiterate, to be operational, an NSM must have two attributes. One, it must have been successfully applied to, and verified for, at least one application and can be used to model another different, but roughly similar, runoff area without extensive internal modification. Two, sufficient written documentation must be available about the model to enable a use to apply the model in a location other than that for which it has been verified.

Relating Problems to Operational Models

Table 3-2 relates the fourteen operational runoff models identified above to the major characteristics which define most runoff problems. The purpose of this table is to provide an efficient manner in which to review the capabilities of the operational models in terms of typical runoff problems which are likely to be encountered in any given REQM analysis.

In the table, seven major problem characteristics--applicable land area, temporal properties, spatial properties, hydrology, hydraulics, quality processes, and residuals--are divided into subheadings. The subheadings enable more distinctions to be made among the capabilities of various models. However, neither the seven major characteristics nor the subheadings within each represent all aspects of runoff problems.

Table 3-2. Applicability of Runoff Models to Various Problem Characteristics

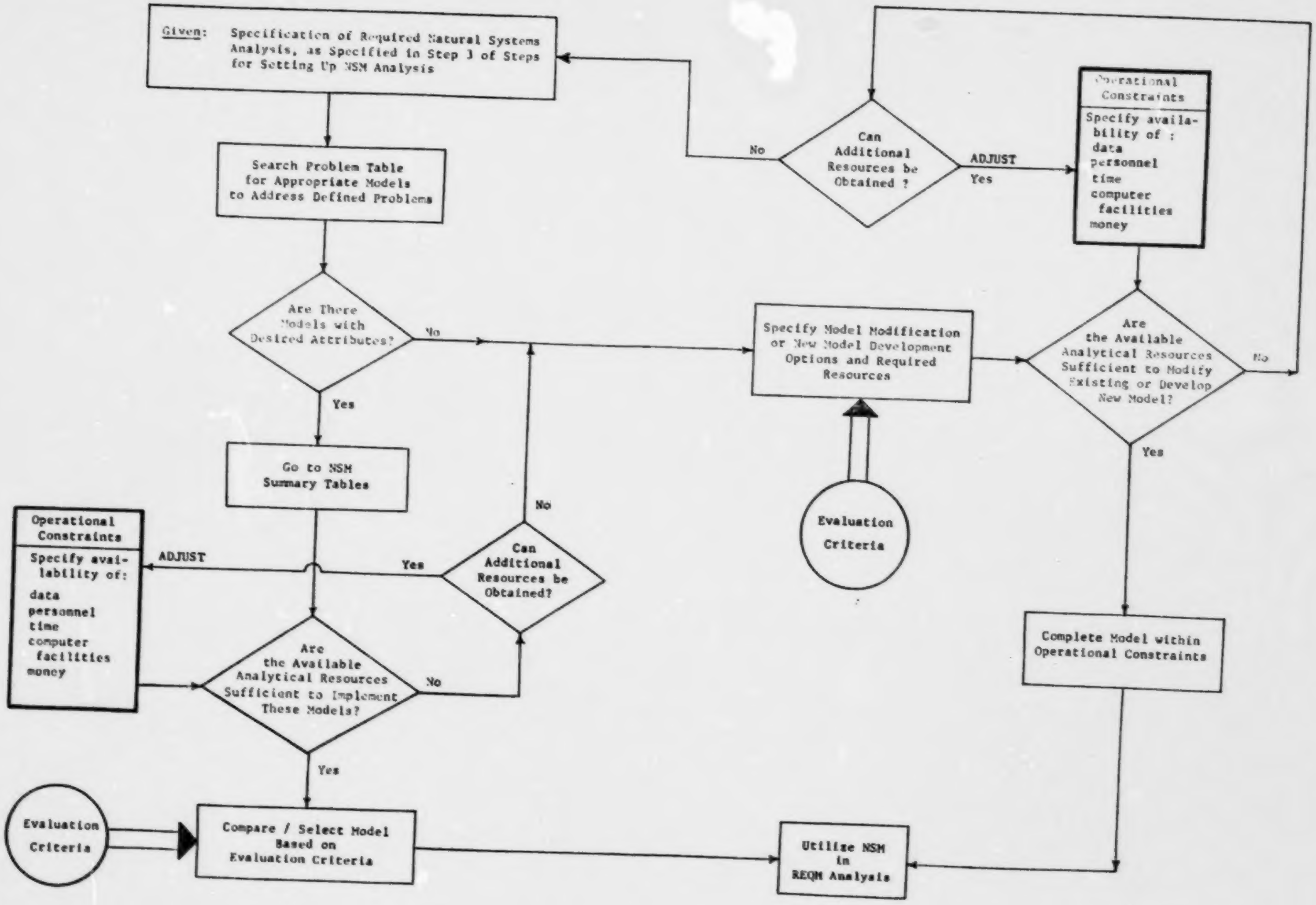
	PROBLEM CHARACTERISTICS																																		
	Applicable Land Area				Temporal Properties			Spatial Properties		Hydrology				Hydraulics				Quality Processes									Residuals								
MODEL NAME	Urban	Agriculture	Forests	Wetlands	Single Storm Events	Continuous Simulation	Annual or Seasonal Average	Single Catchment	Multiple Catchments	Surface/Total Hydrograph Generation	Subsurface Processes	Snowmelt	Dry-weather/Base Flow	Flow Routing in Channels/Pipes	Backwater, Surcharging, Pressure Flow	Flow Controls and Diversions	Storage / Reservoir Routing	Surface Generation	Routing in Channels/Pipes	Sediment / Erosion	Scour / Deposition in Channels/Pipes	Parameter Interaction	Soil/Sediment-Parameter Interaction	Routing through Storages	Treatment/Removal in Storages	Treatment Processes	Organics / BOD / COD	Nitrogen Species	Phosphorus	Suspended Solids	Coliforms	Pesticides	Arbitrary or other Conservative	Arbitrary or other Non-Conservative	Economic Analysis
Hydroscience	●						●	●		●								●						●		●	●	●	●	●	●		●		
MRI	●	●	●				●	●										●		●			●				●	●	●	●	●	●	●	●	
SWMM-Level I	●						●	●		●			●					●									●	●	●	●					●
EPARRB	●	●	●	●	●		●	●										●		●							●	●	●				●		
Simpl. SWMM	●					●			●	●							●									●	●	●	●		●				
ACTMO		●				●			●	●	●	●						●		●	●		●					●	●			●	●	●	
ARM		●			●	●			●	●	●	●								●		●	●					●	●	●		●	●	●	
HSP	●	●	●		●	●			●	●	●	●	●	●		●	●	●	●	●				●			●	●	●	●			●		
NPS	●	●	●	●		●			●	●	●	●						●		●			●				●						●		
QQS	●				●	●			●	●			●	●	●	●	●	●	●					●	●	●							●		
STORM	●					●		●		●		●	●				●	●		●				●	●	●	●	●	●	●	●				
AGRUN		●			●				●	●	●			●				●	●	●							●			●	●		●		
CAREDAS	●				●				●	●			●	●	●	●	●		●					●									●	●	
SWMM	●				●	●			●	●		●	●	●	●	●	●	●	●	●	●			●	●	●	●	●	●	●	●		●		●

Based on this table, an analyst can develop two sets of information. One, for any given problem or set of problems, a number of operational models can be identified. Two, for any given operational model identified in the table, the problems that it can address can be easily identified, and other models capable of addressing the same problems identified. Although problems which models address can be identified using the table, no information can be obtained from the table as to how and with what level of specificity a model can analyze a given problem. Therefore, table 3-2 must be used in conjunction with the model summary tables in Appendix A. Given a number of models of interest identified by means of table 3-2, the model summaries in Appendix A then provide the requisite details about each model. Both table 3-2 and the model summary tables are integral parts of the procedure for selecting a runoff model.

Procedure for Selecting a Runoff Model

The procedure for selecting a runoff model is directly tied to steps four and five in the section on setting up the natural systems analysis in chapter 2. Given that the natural systems analysis required in a given context has been specified--in terms of requiring the analysis of residuals discharges from one or more types of land surfaces. The analyst would then follow the procedure described herein to select an appropriate runoff model. The procedure indicates the questions which must be asked and the activities which must be undertaken before an appropriate model can be selected, given operational constraints. Further, the procedure is the vehicle that operationally integrates this chapter's various sections; it is presented in figure 3-14. Note that the procedure is identical to the flow chart of the NSM selection process contained in chapter 2 (figure

Figure 3-14. Procedure for Selecting a Runoff Model


Given: Specification of Required Natural Systems Analysis, as Specified in Step 3 of Steps for Setting Up NSM Analysis
Search Problem Table for Appropriate Models to Address Defined Problems
Are There Models with Desired Attributes?
No
Yes
Go to NSM Summary Tables
Operational Constraints
Specify availability of:
data
personnel
time
computer facilities
money
ADJUST
Yes
Can Additional Resources be Obtained?
No
Are the Available Analytical Resources Sufficient to Implement These Models?
No
Yes
Evaluation Criteria
Compare / Select Model Based on Evaluation Criteria
Utilize NSM in REQM Analysis
Can Additional Resources be Obtained ?
No
ADJUST
Yes
Operational Constraints
Specify availability of :
data
personnel
time
computer facilities
money
Specify Model Modification or New Model Development Options and Required Resources
Evaluation Criteria
Are the Available Analytical Resources Sufficient to Modify Existing or Develop New Model?
No
Yes
Complete Model within Operational Constraints

2-6) and the procedure for selecting a receiving water model in chapter 4 (figure 4-10). The procedure for selecting an atmospheric quality model is slightly different.

Given that the required natural systems analysis has been specified, the procedure begins with a search of the problem table. If one or more candidate models is or are identified in the table, the analyst then goes to the summary tables to obtain and tabulate the relevant information for each candidate model. For example, table 3-3 is the model summary table prepared for the Agricultural Runoff Model. Descriptions of the characteristics of this table pertaining to all NSMs are in chapter 2. Additional points relating to those characteristics in relation to runoff NSMs and descriptions of characteristics applicable solely to runoff NSMs are contained in the next section.

Next, the available analytical resources to utilize the models are compared with the resources required. If several models can be applied within the operational constraints, then a model is selected on the basis of the evaluation criteria discussed in chapter 2. If only one model can be applied within the operational constraints, then that model would be chosen, unless it does not meet some evaluation criterion deemed critically important.

If no candidate model can be applied within the operational constraints, the logical first option is to attempt to increase the available analytical resources to the level equal to those required to apply at least one of the candidate models. If the additional resources cannot be obtained or if no models can be located in the problem table which are capable of addressing the problems of concern, the analyst has three choices.

Table 3-3. Summary of the Agricultural Runoff Model (AGRUN)

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Agriculture: (a) crops, (b) pasture
Time Properties	(1) Single runoff event simulation; (2) Inputs: precipitation data at 15 minute intervals, daily data for other parameters; (3) Outputs: simulation of time history results based on 15 minute intervals
Space Properties	(1) Small to large multiple catchments; (2) Dimensionality: (a) multiple dimensions: two-dimensional land surface, three-dimensional subsurface layers, one-dimensional stream channel; (3) Discretization limits: (a) watershed may be divided into as many as 200 subareas, (b) subareas may vary in size, (c) tributary drainage system may have up to 200 channels in dendritic pattern (lengths and cross sections can vary), (d) can handle up to 5 soil layers
Physical Processes	(1) Overland flow across land surface and in small stream channels; (2) Groundwater interflow; (3) Channelized tributary flow; (4) Sediment erosion estimated with Universal Soil Loss Equation
Chemical Processes	(1) Constituent transport limited to sediment-attached parameters; (2) All constituents considered conservative--no interaction or degradation; (3) Constituents represented: total suspended solids, BOD, and fecal coliforms are operational
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	Using numerical integration of differential equation set
Computational Status	(1) Coded in Fortran IV; (2) Requires IBM 360/365 digital computer or equivalent; (3) Computer core storage requirements unspecified, but extensive
Input Data Requirements	(1) Precipitation data and drainage channel specifications; (2) Land use hydrogeometric data; (3) Watershed and soil characteristics
Ease of Application	(1) Nonproprietary model derived from SWMM Runoff Module; (2) Basic SWMM documentation available from NTIS or EPA Planning Assistance Branch, Washington, D.C.; (3) Documentation report from Iowa-Cedar River Basin Project available from Water Resources Engineers, Walnut Creek, Ca. or EPA Systems Development Branch, Washington, D.C.; (4) Extent of documentation: (a) SWMM documentation fairly complete for most applications, (b) AGRUN report presents brief information on model modifications, data deck design, sample input and output formats, but no program listings
Output and Output Format	(1) Print of model inputs; (2) Rainfall hyetograph (rate vs. time history) by catchment; (3) Time history of runoff in user-specified stream channels; (4) Time history of sediment concentration in user-specified stream channels; (5) Time history of constituent concentration in stream channels
Linkages to Other Models	(1) Designed to link with nonsteady state receiving water models; (2) Hydrologic linkages result from tributary channel inputs and groundwater inputs (interflow); (3) Final tributary channel output serves as input to receiving water model
Manpower Needs	(1) Environmental engineer experienced in water resources and water quality modeling; (2) Familiarity with Storm Water Management Model and its application useful
Costs	(1) Model acquisition costs are unknown; (2) Program listings could probably be obtained from WRE--Walnut Creek or EPA Planning Assistance Branch for a nominal reproduction charge; (3) Data preparation costs: actual computational costs are unknown
Model Accuracy and Sensitivity	(1) AGRUN can closely simulate watershed with numerous different fields and crop types; (2) Constituent transport limited to sediment-adsorbed substances; (3) No constituent interactions permitted--assumption probably valid if residence time in channels short; (4) No quality constituent (dissolved) transport permitted in groundwater interflow; (5) Rainfall intensity assumed to be uniform over each subcatchment
Other Comments	(1) Only sediment-attached residuals can be simulated; (2) Model originators: (a) AGRUN is a derivative of SWMM for nonurban applications, (b) AGRUN was developed by Water Resources Engineers, Walnut Creek, Ca. for EPA Systems Development Branch, Washington, D.C.

Note: This table also appears in Appendix A as Table 3A-12.

First, the literature can be searched to locate operational models, not included in this table, which will satisfy the analysis requirements. In order to choose among any additional models discovered--in relation to operational constraints and the evaluation criteria--information comparable to that contained in the model summary tables in Appendix A is required. Second, modifications could be made to an existing model to satisfy analytical specifications, given operational constraints and the evaluation criteria. Third, a new model could be developed from "scratch." The second and third choices are shown in the procedure; the first is not. The possibility will always exist that there are models--passed over in the literature--which, when investigated, could be suitable in a given context. If one, two, or three cannot be accomplished due to operational constraints, the evaluation criteria, or lack of knowledge, then the required runoff analysis, i.e., questions to be answered must be respecified and the procedure repeated.

Developing a new model from scratch entails basic theoretical mathematical formulation, debugging after initial set up, sensitivity testing, calibration, and verification. These together represent a level of effort considerably above that involved in applying an existing operational model. Model development requires certain specialized technical skills and substantial resources. It should be undertaken in an REQM analysis only after very careful consideration.

Finally, the procedure described above should not be viewed only in terms of the information presented in this chapter. The activities and questions identified in the procedure are relevant for selecting a runoff NSM under any analysis conditions.

A few additional comments on model selection based on experience in the use of runoff models (Huber, Heaney, and Torno, 1977) are warranted. These comments are generally relevant to all NSMs, not just to runoff models.

First, no intelligent model selection can be performed without a clear statement of the problem at hand and an idea of how and why a model is required. In many cases, standardized engineering analysis techniques may suffice without need for recourse to an unfamiliar model.

Second, experienced personnel, who understand both the physical phenomena being modeled and the model itself, must be employed. Models are never a replacement for engineering skill and judgment. In addition, modeling studies are labor intensive; computer costs are usually in the 10 to 20 percent range of total NSM analysis costs. Experienced personnel are thus more important than the choice of a particular model. For this reason, proprietary models should not be dismissed lightly, because expert assistance is one of their most important attributes.

Third, in almost all cases, the simplest model that will answer the question(s) posed should be used. The value of additional model details and "features," however potentially useful, is seldom worth the additional cost and effort of implementation. Furthermore, additional model complexity usually means additional data requirements and additional costs.

Fourth, it is rare to find a model that does not have programming "bugs" or even outright errors. However, no modification should be made to a model unless absolutely necessary. Modifications are expensive and time-consuming and have a tendency to become ends in themselves, obscuring the original problem. A model user must be prepared to accept the principle of caveat emptor--"let the buyer beware."

Given the selection procedure and the above comments, it is clear that an analyst must ask many questions about individual models before making a selection. For example, is there adequate documentation as to theory, coding, program usage, and example applications? Is the model currently being maintained by a group responsible for corrections and improvements? Is help available to the potential user? Are data requirements realistic within the problem context? The next section describes the types of information needed to answer these and other questions about runoff models.

Definition of Characteristics Used to Summarize Runoff Models

Table 3-3 illustrates the way in which operational runoff models are summarized in Appendix A. Seventeen characteristics are shown for which information on operational models is provided. Chapter 2 stated that these characteristics represent the most important types of information about NSMs, information which is important to know in order to select an appropriate model in a given context. Nine of these characteristics--computational status, input data requirements, ease of application, output and output format, linkages to other models, manpower needs, costs, model accuracy and sensitivity, and other comments--are described in chapter 2, because they are defined similarly regardless of the type of NSM. This is not true of the remaining eight characteristics; hence they are defined here. Also, where relevant in relation to runoff models, some specific comments are made about the characteristics defined in chapter 2.

Applicable Land Drainage Area

This characteristic identifies the type of land area in which a runoff model is applicable in relation to type of land use. As indicated earlier, runoff models can be broadly classified as urban or nonurban. However, this partitioning is not detailed enough because some so-called "urban" models can consider land uses not typically urban, such as agriculture, and vice versa. Further subdivision is required.

For example, urban land can be further divided into residential, commercial, industrial, and open space land use categories. The residential category is the most important one and is often broken down further into high, medium, and low density, or single and multiple family dwellings. Nonurban land use is generally subdivided into agriculture, silviculture, and mining. Within the agricultural category, land use is further divided into irrigated or nonirrigated, and by type of use, e.g., crops, pasture, rangeland.

Time Properties

There are three ways in which time is considered in runoff models: (1) seasonal or annual average; (2) continuous simulation, with a relatively short time step of typically one hour or one day;[19] and (3) single event simulation with time steps of seconds or minutes. In any given context where runoff-related problems are to be thoroughly analyzed, the preferred procedure is to use all three types of models in sequence, i.e., 1, 2, then 3. The simple seasonal or annual average models would provide a general perspective on the problem. Given the resulting rough estimate, a continuous simulation would be used to estimate the dynamic variability of residuals generation from the land surface over a period comprised of multiple storm events. This information would then be used to rank the individual events so that one or more specific single events could be selected for more detailed analysis, given the input conditions for the single event obtained from the continuous simulation.

The requisite temporal properties of a runoff model in any context depend on the receiving water analysis that is to be undertaken. For example, it is unnecessary to utilize a continuous or single event simulation model if what is needed is the analysis of annual nutrient input into a lake.

Space Properties

Space properties of runoff models must be considered in three dimensions, because they either explicitly or implicitly take into account subsurface flow as well as surface flow. Another important spatial aspect relates to the catchment size a model can analyze and whether or not multiple catchments can be considered. An operational classification of catchment sizes is:

Category	Size Range: Acres
Small	< 50
Medium	50 - 500
Large	> 500

This classification is used in the model summary tables.

Catchment size is important because as the size of a catchment increases, it becomes more important to include the effect of flow routing on quantity and quality. On the quantity side, flow routing creates a storage effect in that the hydrographic peak is attenuated and the duration of the runoff event increases. A similar effect is observed in quality as concentration variability is reduced. As a very crude rule of thumb, routing effects should be considered when drainage areas are greater than 50 acres.

Physical, Chemical, and Ecological Processes

These three characteristics were discussed in the section on major natural processes. However, two points relating to how runoff models consider aspects of the physical transport phenomenon merit discussion.

First, the most complicated part of presently available runoff models is the component which deals with analyzing runoff routing through pipe or channel networks. At one end of the spectrum are complex models which require sophisticated numerical integration methods to solve the differential equations used to explain water flow through the system. Such detailed models are frequently employed in the design of water distribution networks and sewers. At the opposite end of the spectrum are simple runoff models which do not include flow routing at all; inflows are assumed to leave the study area during the same time step. This assumption can be very misleading, especially for large catchments where actual travel times may be several times the time step used in the model. It is relatively easy to estimate the time of concentration for the catchment to determine if this type of problem exists. If there is a problem, then a more sophisticated model with a routing capability should be used.

Second, residuals loading data--the types and amounts of residuals which accumulate on and wash off the land surface--are usually based on measurements made on relatively small catchments, i.e., 1 to 10 acres. The portion of the estimated load which eventually reaches a receiving water body is estimated by: either (1) assuming all the load reaches the receiving water body; (2) attenuating the load using a coefficient, i.e., a delivery ratio; or (3) actually modeling the dynamics of the transport process. Most models which analyze agricultural areas employ a delivery ratio. Most models of urban areas assume that all washed off material reaches the outlet of the catchment, because sewers are generally designed to be self-cleaning. However, deposition and scour in sewer systems can be a particularly difficult but relevant problem to consider, especially in combined sewer systems. At present, modeling of scour and deposition can only be done indirectly, by checking pipe velocities from the flow routing analysis.

Many urban runoff models also contain provisions for analyzing various storage and modification options, although the distinction between storage and treatment is somewhat "fuzzy" because modification does occur in storage reservoirs and basins, e.g., settling. Storage facilities reduce the flow variability of the runoff hydrograph. They are widely used for reduction of flood flows and drainage in urban and nonurban areas. Facilities which modify the quality of stormwater range from high rate chlorination to a combination of sedimentation and biological treatment.

Economic Analysis

This characteristic is unique to urban runoff models. It is included because many of the simpler urban runoff models include cost analysis procedures or subroutines. These procedures enable computation of the least cost combination of stormwater management options, given specified criteria. This characteristic is important to identify because: (1) depending on the context, utilizing a runoff model which contains certain economic analysis capabilities could be preferred over using an analogous model which does not; and (2) the extent and type of economic analysis procedures contained in urban runoff models vary.

Linkages to Other Models

Runoff models must be closely linked to both receiving water NSMs and models of residuals generating activities. The former are discussed in several places in the chapter; the latter require additional explanation.

All activities are linked in one way or another to runoff models simply because activities occupy the land surface. However, it is more important to be cognizant of the linkages for some activities than for others. This is particularly true of activities such as agricultural activities for which variables related to the production process also directly affect the quantity and quality of runoff--for example, variables such as type of crop, tillage method, types and amounts of fertilizers and pesticides applied. Consequently, assumptions made regarding these variables in the activity analysis are inputs into the runoff analysis. These assumptions may or may not be consistent with any given runoff model.

Concluding Comment on Model Selection

The foregoing discussion has indicated the requisite steps for choosing a runoff model for a given application. The procedure is applicable regardless of the context. The characteristics which have been chosen to summarize the runoff models contained in Appendix A are useful as a "blueprint" for summarizing all runoff models. As additional models become operational, they can be summarized in the format presented herein and added to Appendix A.

Germane to any discussion of model selection is identification of the problems which relate to model application. An understanding of these problems enables more intelligent use of the information available on NSMs--in this report and existing elsewhere--for selecting an appropriate

NSM. The last section in chapter 2 describec the major problems relating to present applications of natural systems models. These problems are generally relevant for all categories of NSMs and should be reviewed before making final model selection.

GLOSSARY

Adsorption isotherm: At constant temperature, the amount of material adsorbed is a function of the concentration of adsorbate. The functional relationship is called the adsorption isotherm. (See Metcalf and Eddy, 1972.)

Availability factor: Proportion of the residuals load available for washoff in a given time period.

Backwater effects: Propagation of downstream changes in upstream direction, for example, because of a flow modifying structure.

Base flow: Receiving water flow due to groundwater inputs during dry period.

Causation: The independent change in the value of one variable causes a predictable change in the value of dependent variables. The general nature of the functional form can be derived from known physical, chemical, and biological laws.

Coefficient method: Output, e.g., runoff, is a constant fraction (the coefficient) of input, e.g., rainfall.

Contact load: Rolling or sliding of solids along the channel bed.

Dendritic: Branching pattern, as in the limbs of a tree.

Depression storage: Relatively small surface depressions which act as storage areas to collect precipitation and other losses such as interception, initially subtracted from the volume of precipitation in a given precipitation event.

Dry-weather flow: Flow in sewers as a result of all activities other than storm runoff.

First flush: Relatively high concentrations of residuals in the initial runoff during a storm event.

Hydraulic radius: Cross-sectional area of flow divided by the wetted perimeter.

Hydrograph: Figure showing water discharge as a function of time.

Hyetograph: Figure showing rainfall intensity as a function of time.

Impervious area: Land surface through which water cannot infiltrate.

Implicit: Numerical scheme in which a set of simultaneous equations must be solved.

Infiltration: Precipitation penetrating the land surface.

Interception: Volume of water lost from rainfall because of entrapment by vegetation.

Interflow: Infiltrated water that reappears in stream channels without first reaching the zone of saturation.

Invert: Bottom surface of inside of conduit.

Kinematic wave approximation: Solution of one-dimensional momentum and continuity equations neglecting dynamic terms and thus able to include backwater effects. (See Eagleson, 1970.)

Load: Either total mass of residual or mass per unit time, e.g., either total kg or kg/sec.

Loading: Mass of residual per unit area of catchment, sometimes also per unit time.

Manning's roughness: Coefficient, "n", used in Manning's equation to characterize surface roughness. (See Chow, 1959.)

Method of characteristics: Method of analysis of solving kinematic wave problems and Saint Venant equations. (See Eagleson, 1970.)

Nonuniform: Flow conditions are a function of location.

Pervious area: Land surface through which water can infiltrate.

Plug flow: Pure advection--the first residuals to enter a system are the first to leave it.

Pollutograph: Figure showing pollutant concentration or load as a function of time.

Potency factor: Fraction of either total solids or suspended solids (SS) that consist of a particular residual. For instance, if $BOD_5 = 0.005 \times SS$, then the potency factor for BOD_5 is 0.005.

Precipitation event: The amount of precipitation falling during a period beginning with a positive precipitation value in the first time period and ending when zero rainfall has been recorded for a user-specified number of time periods.

Production function: The maximum output attainable from a combination of inputs.

Proprietary model: Model which can be used by contractual arrangement with model developer but is not otherwise available.

Rainfall excess: Rainfall minus losses due to depression storage and infiltration.

Rill Erosion: Erosion from very small channels formed on the land surface.

Saint Venant equations: Momentum and continuity equations describing one-dimensional, transient, free surface flow. (See Chow, 1959.) The two equations may be solved for two unknowns, e.g., velocity and depth.

Saltation load: Movement of solids along the channel bed in short jumps.

Sediment delivery ratio: Proportion of sediment load from a given land area reaching the receiving water.

Sheet erosion: Erosion from land surface associated with overland flow.

Sublimation: The transformation of a material from a solid state directly into a gaseous state without first passing through a liquid state. Sublimation requires both the heat of fusion and vaporization.

Surcharging: Pressure flow in pipe system; that is, water surface above sewer crown.

Time of concentration: Equilibrium time of catchment, that is, the time at which entire catchment contributes to runoff at the outlet. (See Overton and Meadows, 1976.)

Unit Hydrograph: Hydrograph resulting from a rainfall of specified duration producing one inch of runoff. (See Viessman, et al., 1977.)

Volatilization: Removal by vaporization.

Wash load: Solids primarily remaining in suspension in fluid.

Washoff: Removal of residuals from land surface by overland flow.

NOTES

[1] Residuals concentrations in water moving over the land surface are important only in so far as that information is needed to estimate residuals concentrations in runoff as the runoff enters a receiving water body, or for analyzing residuals discharge reduction measures.

[2] The term "solids" is not well defined; it denotes any of several types of soluble and insoluble residuals.

[3] Runoff models frequently employ a one-dimensional analysis of advection and diffusion using conservation of mass and energy principles. This is discussed further in the section on analytical approaches.

[4] A conservative residual is a residual which does not decay during the process of transport; a nonconservative residual decays during transport.

[5] Some sections of some urban areas, such as major parks, are comparable to nonurban areas with respect to factors affecting runoff. For those sections, nonurban type runoff models might be appropriate.

[6] In Great Britain, the rational method is known as the Lloyd-Davies method.

[7] The conversion 1.0 in/hr approximately equal to 1.0 cfs/acre is used to obtain Q in cfs.

[8] Applications of this approach include Snyder (1938), Eagleson (1962), Morgan and Johnson (1962), Espey, Morgan, and Mach (1965), Betson and Green (1968), Hamm, Morgan, and Reeder (1973), and Brater and Sherrill (1975).

[9] An instantaneous unit hydrograph is equivalent to an impulse response in systems theory.

[10] For example, for some purposes, such as developing inputs to simulation models, a variable--e.g., runoff or rainfall--may be treated as a time series and alternative future possible sequences of runoff or rainfall events generated on the basis of preserving certain statistics of its past history, e.g., mean, standard deviation, skewness. Markov models are examples. (See Fiering and Jackson, 1971.) Other techniques are described by Ciriani, Maione, and Wallis (1977). Also, hydrologic characteristics may be treated as random variables and analyzed probabilistically. The resulting probability density functions are then used in frequency analyses. These techniques and others are covered, for example, by Haan (1977).

[11] For examples of solutions of the equations of motion, see Morgalia and Linsley (1965).

[12] For a complete derivation, see pp. 6-7 in Rovey, Woolhiser, and Smith (1977).

[13] For example, classical work has been performed using the kinematic wave formulation by Henderson and Wooding (1964), Wooding (1965a, 1965b, 1966), and Woolhiser and Ligget (1967). Good explanations of the features of kinematic waves are given by Eagleson (1970), and Overton and Meadows (1976). Many applications exist, including Harley, Perkins, and Eagleson (1970), Bras and Perkins (1975), Singh (1975), and Woolhiser (1972a).

[14] It should be emphasized that these approaches are comprised of more explicit, process-oriented models than is the rational method.

[15] For example, see Soil Conservation Society of America (1976), Vanoni (1975), and U.S. Department of Agriculture (1975).

[16] Other statistical methods employed include standard correlation analysis and spectral analysis. For example, see Thomann (1972) and Wastler (1969). Probability theory can also be used to construct probability distributions of residuals concentrations in runoff, distributions which are altered as residuals pass through control devices on their way to receiving waters. The altered probability density functions may be derived analytically, assuming simple transfer functions for conversion of inflow to outflow concentrations. Such an approach is given by the Environmental Protection Agency (1976).

[17] For a discussion of other limitations of the USCE, see El-Swaify, Dangler, and Armstrong (1979).

[18] The population compiled for runoff models includes numerous simplified models under the headings "screening procedures" and "simplified computer models," which can be used for preliminary analysis. This is not the case in the other NSM chapters. Note also that some models may encompass more than one category.

[19] Continuous simulation models applied to pervious areas have the advantage that they can account for changes in soil moisture and for the accumulation and degradation of residuals on the land surface.

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Appendix A

MODEL SUMMARY TABLES

Table 3A-1. Summary of the Hydroscience Simplified Model

Characteristic	Summary Data
Applicable Land Drainage Area	Urban
Time Properties	Average annual inputs and outputs
Space Properties	Small to large single catchment
Physical Processes	(1) Rainfall/snowmelt runoff estimated by coefficient method; (2) Wet-weather quality assumed to have constant concentration; (3) No treatment is assumed to occur in storage; (4) Treatment is simply a hydraulic accounting of flow-through capability, no explicit residuals discharges removal
Chemical Processes	(1) Quality constituents input at constant concentration; (2) Suspended solids, BOD, COD, nitrogen, phosphorus, and lead are represented
Ecological Processes	Fecal coliforms are represented
Economic Analysis	None
Mathematical Properties	Statistical model with graphical solution
Computational Status	Calculations can be performed with hand-held calculator
Input Data Requirements	Mean rainfall intensity, runoff coefficient, drainage area, variation in rainfall intensity, storage volume, interception capacity, residuals discharge concentrations
Ease of Application	(1) Nonproprietary model; (2) Procedures are documented; (3) User support available through Hydroscience: (4) Limited user experience to date
Output and Output Format	Output is expected effectiveness of reservoir and interceptor (treatment) units
Linkages to Other Models	Linked to Hydroscience Simplified Receiving Water Model
Manpower Needs	Environmental engineer familiar with statistics
Costs	(1) Model is available free of charge; (2) Precipitation data tapes available from U.S. Weather Bureau for about $100; (3) Land use data usually available at little cost; (4) No computer related expenses involved
Model Accuracy and Sensitivity	(1) Relatively crude model; (2) Could be interfaced with continuous simulation models to calibrate performance curves; (3) Neglects treatment in storage
Other Comments	(1) A simple model which is quite useful for preliminary screening; (2) Model developed by Hydroscience, Inc., Westwood, N.J. under EPA sponsorship

Table 3A-2. Summary of EPA Storm Water Management Model: Level 1 (SWMM-Level I)

Characteristic	Summary Data
Applicable Land Drainage Area	Urban
Time Properties	Average seasonal or annual inputs and outputs
Space Properties	Small to large single catchment
Physical Processes	(1) Runoff estimated as a function of population density and precipitation; (2) Dry-weather flow quantity estimated by coefficient method; (3) Wet-weather quality estimated as a function of land use, precipitation, population density, type of sewerage system, and street sweeping frequency; (4) Effectiveness of storage/treatment evaluated by deriving production function, regionalized parameters are used; (5) Street sweeping production function is included; (6) Sewer flushing production function is included
Chemical Processes	(1) Quality constituents are represented as conservative substances; (2) BOD_5, SS, VS, PO_4 and N are represented
Ecological Processes	None
Economic Analysis	Provides the least costly combination of storage/treatment and other management practices
Mathematical Properties	Deterministic model with graphical or analytical solution of algebraic equations
Computational Status	Calculations can be performed with hand-held calculator
Input Data Requirements	Precipitation, land use, population density, type of sewerage system, street sweeping frequency, treatment efficiencies, control costs
Ease of Application	(1) Nonproprietary model; (2) Two documentation reports available through EPA or University of Florida; (3) Documentation includes example problems; (4) User support available through University of Florida and EPA workshops; (5) Used extensively in nationwide assessment, needs surveys, and EPA 208 studies throughout the U.S.
Output and Output Format	No specified output format
Linkages to Other Models	Part of overall EPA SWMM package
Manpower Needs	Environmental engineer with some background in economics
Costs	(1) Nominal setup costs; (2) No computer related expenses involved
Model Accuracy and Sensitivity	(1) Relatively crude model; (2) Provides a rough check on the reasonableness of simulated results for a given area; (3) Neglecting treatment in storage may mislead users into specifying two separate control units when a single storage/treatment unit could be used
Other Comments	(1) Popular model that has been used extensively; (2) User support available; (3) Model developed by the University of Florida, Department of Environmental Engineering, under EPA sponsorship

Table 3A-3. Summary for the Midwest Research Institute (MRI) Nonpoint Source Loading Functions

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Urban and suburban; (2) Agriculture: irrigated and non-irrigated; (3) Silviculture or natural forests
Time Properties	(1) Annual average; (2) Input usually annual averages; (3) Output on daily and monthly basis
Space Properties	Small to large single catchment
Physical Processes	(1) Hydrology not considered directly; (2) Sediment erosion predicted by the Universal Soil Loss Equation
Chemical Processes	(1) Transport of most constituents as sediment-attached particles; (2) Constituents represented: (a) nitrogen (adsorbed species only), (b) phosphorus, (c) BOD/organic matter, (d) pesticides, (e) salinity, (f) radioactivity, (g) heavy metals, (h) coliforms, (i) sulfur compounds (from acid mine drainage)
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	Deterministic model using analytical solution of algebraic equations
Computational Status	Calculations can be performed with hand-held calculator
Input Data Requirements	(1) Model input data: (a) areal characteristics--location, size, land use categories, (b) USLE factors--source area, rainfall, soil erodibility, slope length, slope gradient, cover, practices, and sediment delivery ratio, (c) enrichment factors for erosion of various constituents, (d) concentration of constituents in soil or runoff; (2) Model verification data: (a) not applicable
Ease of Application	(1) Nonproprietary model; (2) Loading function documentation report available through EPA Office of Research and Development, Washington, D.C. or NTIS, Springfield, Va.; (3) Extent of documentation: (a) theoretical description of loading equations (by constituent), (b) discussion of the computational procedure with examples, (c) appendices (tables and graphs) to provide USLE factors by geographical location
Output and Output Format	(1) Average daily loading of residual from each land use category; (2) 30-day maximum daily loading of residual from each land use category; (3) 30-day minimum daily loading of residual from each land use category
Linkages to Other Models	None
Manpower Needs	(1) Engineering technician or junior-level engineer; (2) Some basic experience in water quality or soil conservation
Costs	(1) Documentation report available from NTIS; (2) No computer-related expenses involved; (3) Model acquisition costs: (a) documentation report available for less than $10 from NTIS; (4) Data preparation costs: (a) supplemental field data collection may be necessary to augment available data base
Model Accuracy and Sensitivity	(1) MRI loading functions do not represent individual processes within the study area; (2) Factors for computation provided for user on geographically-aggregated basis (poor spatial resolution); (3) Limited to sediment-attached constituents for many sources
Other Comments	(1) Loading functions useful as "first cut" estimate of residuals generation only; (2) Technique permits little temporal or spatial variation, or process detail; (3) Model developed by Midwest Research Institute, Kansas City, Mo. for EPA Office of Research and Development, Wash., D.C.

Table 3A-4. Summary of the Environmental Pollution Assessment-Erosion, Sedimentation, and Rural Runoff Model (EPARRB)

Characteristic	Summary Data
Applicable Land Drainage Area	Any nonurban area
Time Properties	(1) Single storm evunt for erosion and sedimentation; (2) Monthly input and output data (may vary if optional single storm event simulated); (3) One to twelve consecutive months may be simulated; (4) Monthly time intervals for model computation
Space Properties	Large, single catchment
Physical Processes	(1) No individual hydrologic processes represented; (2) Erosion and sediment movement are calculated using the Universal Soil Loss Equation
Chemical Processes	(1) Constituent transport is a component of total sediment transport; (2) Constituents represented: (a) BOD, (b) TOC, (c) nitrogen, (d) phosphorus, (e) potassium, (f) acid drainage, (g) forest litter, (h) animal and fowl droppings
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	(1) Stochastic model using random number generator to introduce probabilistic, highly variable conditions; (2) A deterministic system can be obtained by using mean values and zero deviations; (3) Algebraic solution of empirical equation
Computational Status	(1) Coded in Fortran IV; (2) Computer core storage requirements unspecified; (3) Source and library programs operational on EPA-OSI system (disk RIV004)
Input Data Requirements	(1) Control information--starting and ending months, random number generator and multiplier for loads; (2) State data--name of state or number of subunits being investigated; (3) Topographical data--acreage involved and plot size of each land unit; (4) Soils erodibility information for various soil types (max. 5) on each land unit; (5) Slope percentage and slope length (mean and percent deviation) on each land unit; (6) Cropping management factor for each land use category; (7) Erosion control practice factors for each land use category; (8) Sediment delivery and downstream migration factors; (9) Percentage of constituents in delivered sediments; (10) Numbers of livestock and fowl present on each land unit; (11) Forest litter data on each land unit--amount, constituent content, and delivery factor
Ease of Application	(1) Nonproprietary model; (2) Source programs and test run case are available on library disks from EPA-OSI computer system at EPA Region IV, Surveillance and Analysis Division, Athens, Ga.; (3) Documentation report on nonpoint assessment processes also available; (4) Extent of documentation: (a) short description of model theory, (b) data deck design, (c) program listings, (d) appendix tables for various factors required by Universal Soil Loss Equation
Output and Output Format	(1) Tons of soil loss per land unit; (2) Tons of sediment delivered to water bodies per land unit; (3) Tons of sediment migrating downstream; (4) Pounds of constituents contributed by each land unit
Linkage to Other Models	EPARRB is intended for concurrent use with Environmental Pollution Assessment Urban, Commercial, and Industrial Runoff Model (EPAURA)--loadings from both models are summed along with point source loadings to determine total core city, urban, and rural loadings to water bodies (EPATLC)
Manpower Needs	(1) Engineering technician or junior level engineer/planner; (2) Experience with water quality and soil conservation practices useful, but not required
Costs	(1) Model acquisition costs are unknown--likely to be inexpensive due to internal EPA development; (2) Data preparation: (a) much of data taken from USDA Agricultural Handbook appendices and prepared soil and land use maps--little field collection of data required; (3) Actual computational costs are unknown
Model Accuracy and Sensitivity	(1) EPARRB does not consider rainfall and subsequent runoff hydrology--only empirical relationship of erosion resulting from these processes; (2) Sediment and constituent transport also derived from observational data rather than simulation of individual processes; (3) Potential large size of study area distorts model resolution and believability
Other Comments	(1) EPARRB is useful for "first cut" estimations of nonpoint source contributions to receiving water bodies; (2) Model has poor temporal and spatial resolution as well as total lack of process detail; (3) Model originators: (a) EPARRB (as well as EPAURA and EPATLC) developed by Ambient Monitoring Section, Surveillance and Analysis Division, EPA, Athens, Georgia for use in nonpoint source analysis in Section 208 studies

Table 3A-5. Summary of the Simplified Storm Water Management Model (Simplified SWMM)

Characteristic	Summary Data
Applicable Land Drainage Area	Urban
Time Properties	(1) Continuous simulation with hourly time step; (2) Input on an hourly basis; (3) Output by event
Space Properties	Medium to large multiple catchments
Physical Processes	(1) Runoff estimated by coefficient method; (2) Wet-weather quality estimated using regression analysis of local data set; (3) No treatment is assumed to occur in storage; (4) Treatment is simply hydraulic accounting of flow-through capability, no explicit removal of residuals
Chemical Processes	(1) Quality constituents represented as conservative substances; (2) BOD, nitrogen, and phosphorus are represented
Ecological Processes	Coliforms may be represented
Economic Analysis	None
Mathematical Properties	Deterministic model with iterative solution of algebraic equations
Computational Status	(1) Coded in IBM Fortran IV; (2) Operational on an IBM 360/67, storage-treatement components run on a Xerox 560 and an IBM 1130; (3) Storage requirements: 40K of core storage; (4) Input by card reader and/or tape/disk
Input Data Requirements	Hourly precipitation, runoff coefficient treatment rate and storage volume, receiving water characteristics
Ease of Application	(1) Description and documentation available from Metcalf and Eddy, Inc., Palo Alto, Ca., or EPA, Edison, N.J.; (2) Model has been tested on Rochester, N.Y.; (3) Model is available only from EPA, Washington, D.C.; (4) No user support available
Output and Output Format	(1) Tabular listing and a ranking of storm event runoff; (2) Tabular listing of storage/treatment utilization; (3) Tabular listing of runoff quality
Linkages to Other Models	Linked to simplified, single event receiving water model
Manpower Needs	Environmental engineer with some programming experience
Costs	(1) Documentation available at nominal cost; (2) Precipitation tapes available from U.S. Weather Service for about $100; (3) One year simulation costs about $13.00; (4) Set-up costs may be high due to incomplete documentation and no user support
Model Accuracy and Sensitivity	Model provides screening information
Comments	Model developed by Metcalf and Eddy, Inc., Palo Alto, Ca. under EPA sponsorship

Table 3A-6. Summary of Hydrocomp Simulation Program (HSP)

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Urban; (2) Agriculture; (3) Forest
Time Properties	(1) Continuous simulation with hourly time step, run for extended periods, usually a year or more; (2) Time step of input data: (a) precipitation (hourly), (b) air temperature, dew point, solar radiation, and wind velocity (daily); (3) Time units on output: hourly, event, and/or annual summaries
Space Properties	(1) Multiple catchments, overland flow, open channel, and sewer routing with modified kinematic wave formulation using Manning's equation; (2) Does not explicitly handle surcharging, does flag if surcharging occurs; (3) Reservoir routing can be included
Physical Processes	(1) Rainfall/snowmelt runoff estimated by detailed accounting of water balance in upper and lower soil storage zones and deep groundwater zone, incorporates interception, evaporation, and evapotranspiration; (2) Dry-weather flow quantity estimated by coefficient method; (3) Wet-weather quality estimated using linear residuals buildup with washoff rate directly proportional to runoff, separate washoff functions are used for each residuals discharge; (4) Dry-weather quality estimated by coefficient method; (5) Storage routing, no treatment simulation or treatment in storage
Chemical Processes	Quality constitutents represented as conservative substances; suspended and settleable solids, BOD, total nitrogen, and orthophosphate are represented
Ecological Processes	Coliforms are represented
Economic Analysis	None
Mathematical Properties	(1) Deterministic model with iterative solution of algebraic equations; (2) Mathematical representation based on physical concepts but formulations are based largely on empirical relationships
Computational Status	(1) Coded in four main programs; (2) Equipment requirements: IBM 360 and 370 computers or equivalent with at least 240K bytes of core memory
Input Data Requirements	Job specification; hourly precipitation; max-min daily air temperature; daily radiation, cloud cover, dew point, and wind; daily or semi-monthly evaporation; HSP calibration parameters, e.g., infiltration, depression storage, residuals decay rates
Ease of Application	(1) Proprietary model of Hydrocomp, Inc., Palo Alto, Ca.; (2) Current user's manual available for quantity (Jan. 1976) and quality (April 1977); (3) Documentation includes detailed description of the model components and underlying equations and assumptions; (4) Extensive user support available through Hydrocomp which also publishes periodic newsletters and conducts short courses; (5) HSP has evolved from the Stanford Watershed Model which was originally developed for hydrologic simulation of nonurban catchments; it is probably the most detailed and complete rainfall/runoff model and the most widely used quantity simulator model; quality modeling is similar to other models and has been used in recent EPA 208 studies, e.g., Chicago; (6) Model is especially well suited for continuous simulation where detailed hydrologic analysis is needed
Output and Output Format	(1) Flexible output format from quantity and quality analysis including tabular and graphical arrays, routine statistical analysis and frequency analysis; (2) Monthly, annual, and period of record summaries available
Linkages to Other Models	(1) Linked to Hydrocomp's receiving water model; (2) Related models have been developed for agricultural areas, e.g., the Agricultural Runoff Model (ARM)
Manpower Needs	Environmental engineer familiar with hydrology
Costs	(1) Proprietary model of Hydrocomp, Inc., (2) Initial cost to become familiar with program is several hundred dollars to participate in short course, user costs depend on requested level of professional services
Model Accuracy and Sensitivity	(1) HSP is very well suited to problems where continuous simulation is needed with emphasis on quantity; (2) Its quality version has the same residuals discharge buildup and washoff relation as SWMM and STORM
Other Comments	(1) The quantity model has been used extensively; (2) HSP has a very flexible data handling capability; (3) Excellent user support is available

Table 3A-7. Summary of the Agricultural Runoff Model (ARM)--Version II

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Agriculture: (a) crops, (b) pasture
Time Properties	(1) Continuous simulation with variable time step; (2) Precipitation data input at 5-15 minute intervals, but other inputs may be based on daily, weekly, or even monthly data; (3) Output data in 5-15 minute intervals during simulation of storm events and daily values during non-storm periods; (4) Total simulation period dependent upon length of growing season for area of interest
Space Properties	(1) Small to medium multiple catchments; (2) Dimensionality: (a) multiple dimensions--two-dimensional, irregularly-shaped land surface areas, subsurface layers; (3) Discretization limits: (a) size of catchment dependent upon maximum runoff area without formation of channels (varies with site topography), (b) soil profile (3 layers) extends to 6 ft. (1.83 m) depth
Physical Properties	(1) Surface flow produced by precipitation runoff and snowmelt; (2) Subsurface water movements (infiltration, interflow, and percolation loss to groundwater); (3) Interception (vegetative depression storage loss); (4) Snow accumulation and melt (based on ambient energy balance); (5) Surface flow considers both sheet and rill erosion (detachment, pick up, and transport of soil fines)
Chemical Processes	(1) Consist of: (a) sediment, pesticide, and nutrient process submodels; (2) Chemical transport involves both solution phase (dissolved) and sediment-adsorbed constituents; (3) Quality constituents represented: (a) soil fines (silt and clay fraction), (b) pesticides (paraquat, atrazine, and diphenamid tested), (c) nutrients (nitrogen series and phosphorus); (4) Chemical interactions: (a) optional use of non-single-valued adsorption/desorption functions permits different process curves in comparison to a single-valued function, (b) nutrient interactions include first-order rates for immobilization, mineralization, nitrification/denitrification, plant uptake, and adsorption/desorption
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	Deterministic model using numerical integration of differential equation set
Computational Status	(1) Coded in IBM Fortran IV; (2) Operational on IBM 360/67 series; (3) Version II has option to permit operation on Hewlett-Packard 3000 series II (required internal program modification not apparent to the user); (4) Storage requirements unknown
Input Data Requirements	(1) Hydrology--groundwater zone's moisture storage, infiltration rates, percolation to groundwater, interflow storage and rates, hydrogeometric data for overland flow (average slope, Manning's roughness coefficient, distance to channel), evapotranspiration rates, percentage of impervious area; (2) Snow conditions--mean watershed elevation, snow density and water content, conversion temperature from precipitation to snow, initial snowpack depth and water equivalent, temperature affecting potential evapotranspiration (min. and max.), meteorological factors (solar radiation, condensation and convection melt, groundmelt, snow evaporation); (3) Sediment--monthly crop cover (percentage), time of tillage (Julian dates for two years), production of soil fines by identified tillage events, initial fines deposit, daily fines reduction rate on non-rain days, exponents of rainfall intensity and overland flow, coefficients in soil splash and sediment washoff equations; (4) Pesticides--initial pesticide storage in all four subsurface zones, time, mode, and amount of pesticide application, pesticide solubility in water, adsorption and desorption exponents, daily decay rate; (5) Soil conditions--temperatures (monthly) for each subsurface zone, surface layer and upper zone soil depth, bulk density of upper and lower zone soils, chemical percolation factors for both upper and lower zones; (6) Nutrients--timestep of chemical and biological transformations (usually 5-60 minutes), number of fertilizer applications (0-5), time of plant harvest (Julian date), fraction of maximum crop uptake (monthly) of nutrients for the upper soil layers and fraction of lower soil zone; (7) Nitrogen reaction rates--oxidation-reduction rate, uptake, mineralization, immobilization, and adsorption/desorption transfers for ammonium, nitrite, nitrate, and organic N; (8) Phosphorus reaction rates--mineralization, immobilization, uptake, and adsorption/desorption transfers for phosphate, and organic P; (9) Nutrient storages--nitrogen, phosphate, chloride
Ease of Application	(1) Nonproprietary model; (2) Documentation reports available from NTIS, EPA Environmental Research Lab., Athens, Ga., or Hydrocomp, Inc., Palo Alto, Ca.; (3) Extent of documentation: (a) brief theoretical description, (b) brief subroutine descriptions; (c) discussions of parameter evaluations for simulation of soil environment, soil pesticides, soil nutrients, and runoff components, (d) sample input, (e) simulation results on test watersheds, (f) complete model source listings for Version II
Output and Output Format	(1) Monthly summaries for total runoff, total sediment loss, and pesticide or nutrient loss from watershed; (2) Daily (or smaller time interval) simulation of runoff, sediment loss, and pesticide/nutrient loss for single storm event

Table 3A-7. Summary of ARM--Version II (continued)

Characteristic	Summary Data
Linkages to Other Models	ARM produces optional output file for simulated runoff and sediment to be used as input to the receiving water model
Manpower Needs	(1) Junior-level engineer with previous experience in water resources, water quality, and soil conservation/agricultural engineering; (2) Familiarity with HSP-Land Hydrology, PTR, or other similar watershed models useful
Costs	(1) Two documentation reports available form NTIS for nominal cost; (2) Familiarization may take 2-3 man-weeks; (3) Data collection costs increase considerably when pesticide and/or nutrient analyses required; (4) Preparation of model input sequence will require several man-weeks; (5) Parameter evaluations may take 1-2 man-weeks; (6) Actual computational costs are unknown
Model Accuracy and Sensitivity	(1) Considers both dissolved phase and sediment-adsorbed constituents (most realistic description of real-life constituent movement); (2) Non-single-valued adsorption/desorption equations permits better descriptions of soil-chemical interactions; (3) Subsurface water movement, particularly interflow, important to dissolved nutrient simulation; (4) Nutrient transformations permitted by ARM should permit greater resolution of watershed losses
Other Comments	(1) ARM process models for pesticide and nutrient transformation require additional field testing; (2) Sediment production by tillage in different geographic area is needed to refine the relationship between erosion and agricultural practices; (3) Model originators: (a) ARM based on earlier Pesticide Transport Model, (b) model hydrology derived from Stanford Watershed Model and HSP, (c) ARM developed by Hydrocomp, Inc. for EPA Environmental Research Lab., Athens, Ga.

Table 3A-8. Summary of the Nonpoint Source Model (NPS)

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Urban; (2) Agriculture
Time Properties	(1) Continuous simulation; (2) Input: (a) precipitation data at 15 minute or hourly intervals during simulated storm events, daily during non-storm periods; (b) monthly and yearly output; (3) One year simulation recommended but period is optional
Space Properties	(1) Small to medium multiple catchments; (2) Dimensionality: (a) multiple dimensions--two-dimensional land surface, subsurface zones
Physical Processes	(1) Gravity surface flow generated by precipitation runoff and snowmelt; (2) Subsurface infiltration and groundwater interflow; (3) Surface erosion of dust and dirt considered; (4) Snow accumulation and snowmelt also considered
Chemical Processes	(1) Only simulates transport of constituents that are attached to sediment particles--no aqueous phase constituents; (2) Quality constituents represented: (a) temperature, (b) BOD, (c) saturation dissolved oxygen, (d) user may specify up to five sediment-attached constituents (heavy meatals, pesticides, nutrients, etc.)
Ecological Processes	None
Mathematical Properties	Deterministic model using numerical integration of differential equation set
Computational Status	(1) Coded in IBM Fortran IV; (2) Operational on IBM 360 or 37[illegible] series; (3) Requires up to 144,000 IBM byte computer core storage for a normal production run
Input Data Requirements	(1) 15 minute or hourly precipitation, daily potential evapotranspiration, daily air temperature (max. and min.); (2) Parameter evaluation data: (a) hydrology; (2) Groundwater zone storage, infiltration, groundwater seepage or interflow, watershed area, hydrogeometric data (Manning's N, average slope, length to channel) for overland flow on pervious areas, hydrogeometric data for overland flow on impervious areas, evapotranspiration factors; (3) Snow conditions--topographical elevation, snow density and meteorological conditions (solar radiation, temperature, condensation and convection melt, evaporation); (4) Water quality--soil splash and soil washoff features for both pervious and impervious areas; (5) Land use information--fraction of watershed in each land use, features of pervious areas--annual or monthly potency factors, daily accumulation rates, initial sediment accumulation, daily removal rates of sediments, features of impervious areas--potency factors, accumulation and removal rates, initial accumulations
Ease of Application	(1) Nonproprietary model; (2) Documentation reports available from EPA Southeast Environmental Research Lab., Athens, Ga., or Hydrocomp, Inc., Palo Alto, Ca.; (3) Extent of documentation: (a) brief theoretical description, (b) brief subroutine descriptions--MAIN, QUAL, LANDS, (c) individual parameter evaluations, (d) sample model input, (e) descriptive calibration information, (f) source listings available, (4) Supplemental documentation report gives new source listings for model application to nutrient dynamics on small watershed
Output and Output Format	(1) Summary of simulation run characteristics and input parameters; (2) Time interval output and storm summaries--user can specify minimum "trigger" flow to produce output when exceeded, entire watershed values of total flow and quality printed in production run storm output; (3) Monthly and yearly summaries (average, maximum, minimum, range, and standard deviation) for total runoff, peak flow, total residuals washoff, maximum residuals mass washoff, mean residuals concentration, maximum residuals concentration during storm events
Linkages to Other Models	NPS produces output file or tape that is used as input to the HSP receiving water model
Manpower Needs	(1) Junior level engineer with previous experience in water resources and water quality areas; (2) Familiarity with HSP or its derivatives useful
Costs	(1) Documentation reports available from NTIS for nominal cost; (2) Familiarization will take 2.5 man-weeks; (3) Data collection and preparation takes 1 week per year of simulation; (4) Preparation of model input sequence for meteorological data requires 1.5 man-weeks per year of simulation; (5) Model analysis costs: (a) 1 man-week for parameter evaluation, (b) calibration requires 3 man-weeks per year of simulation; (6) Actual computational costs are unknown
Model Accuracy and Sensitivity	(1) All quality constituent transport related to sediment movement; (2) NPS simulations represent adsorbed constituents relatively well, but lack ability to simulate accurately constituents which are transported totally or partially in the aqueous phase
Other Comments	(1) NPS only handles constituent transport when linked to sediment transport; (2) Model originators: (a) model hydrology derived from Stanford Watershed Model and HSP-QUALITY, (b) NPS developed by Hydrocomp, Inc., for EPA Environmental Research Lab., Athens, Ga., (c) erosion processes simulated with Universal Soil Loss Equation

Table 3A-9. Summary of the Agricultural Chemical Transport Model (ACTMO), Using USDAHL-74 Watershed Hydrology

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Agriculture: (a) crops, (b) pasture
Time Properties	(1) Continuous simulation with hourly time steps; (2) Input precipitation data at hourly intervals, data between storms can be daily, weekly, or monthly; (3) Output daily summaries during storm events, weekly or monthly summaries at other times
Space Properties	(1) Small to medium multiple catchments; (2) Dimensionality: (a) multiple dimensions: two-dimensional land surface (divided into zones and tubes), subsurface layers; (3) Discretization limits: (a) usually four subsurface layers used (plow layer, potential root zone, 2 storage zones), (b) size of tube area related to the average zone length and the fraction of zone area that contributes directly to the channel, (c) usually 3 or 4 zones that contribute to a stream channel are utilized
Physical Processes	(1) Downslope surface flow moves across each zone toward a stream channel following rainfall event or snowmelt; (2) Subsurface infiltration and groundwater interflow; (3) Evapotranspiration loss; (4) Infiltration and interflow; (5) Snow accumulation and melt; (6) Rill and interrill erosion based on the Universal Soil Loss Equation
Chemical Processes	(1) Adsorption, breakdown, dispersion, transport (via infiltration, runoff, rill, and interrill erosion, lateral outflow), deposition, mineralization, plant uptake for agricultural chemicals; (2) Quality constituents represented: (a) agricultural chemicals, particularly pesticides and fertilizers, (b) nitrates produced by microorganisms (optional); (3) Only one chemical type or application at a time is simulated
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	Deterministic model with unspecified solution technique
Computational Status	(1) Nonproprietary model coded in Fortran IV (G level); (2) Operational on IBM 360 or 365 series computer or UNIVAC 1108 (using Exec 9 control language); (3) Requires 98,000 bytes of storage capacity on IBM system or 19,000 word storage capacity on UNIVAC system; (4) Fortran G level compiler necessary
Input Data Requirements	(1) Watershed characteristics (for each compartment)--soil erodibility factor, slope steepness (percent), length of overland flow (ft.), compartment width (ft.), surface texture, crop factor, management factor, soil layers and subsurface parameters; (2) Chemical information--date of application, application rate (lbs./acre), depth of mixing (in.), adsorption coefficient (ratio of concentration), breakdown coefficient (loss/day), relative preference for size fractions; (3) Physical data--dispersion distribution factor (in.), field capacity (%), soil porosity (%), soil texture; (4) Hydrological data--storm data, infiltration (in.) before and during runoff, runoff (in.) before and during runoff, runoff (in.), ratio of lateral to vertical flow, soil moisture at start of storm, cascading parameters; (5) Erosion data--interrill erosion (tons), rill erosion (tons), fraction of area in rills, rill depth (in.), sediment deposition (tons), sediment texture
Ease of Application	(1) Nonproprietary model; (2) Description report available as ARS-H-3 from U.S. Dept. of Agriculture, Agricultural Research Service, Hyattsville, Md., USDAHL-74 hydrology model documentation report also available from ARS, Hyattsville, Md. as Technical Bulletin No. 1518; (3) Extent of documentation: (a) brief theoretical description, (b) no subroutine descriptions (ACTMO), (c) USDAHL-74 report provides sample input parameter, sample output files, subroutine flow diagrams, and program listings; (4) Both ACTMO and USDAHL-74 reports needed for successful application; (5) ACTMO application from available reports likely to be difficult due to sketchy instructions
Output and Output Format	(1) Streamflow data illustrating storm hydrograph taken at 15 min. intervals; (2) Daily water budget summaries for runoff and terrestrial system zones; (3) Monthly and annual summaries of system water budget; (4) Total watershed erosion by storm event; (5) Total quantity and runoff concentrations of agricultural chemicals; (6) Quantity of water sediment, and chemicals in each model compartment during selected storm
Linkages to Other Models	(1) ACTMO is a composite model consisting of USDAHL-74 model for system hydrology, Universal Soil Loss Equation for erosion, and a chemical model
Manpower Needs	(1) Computer programmer and engineer with experience in water resources, soils science, water quality, and/or agricultural engineering; (2) Familiarity with USDAHL-74 hydrology model is essential to set up and apply ACTMO
Costs	(1) Documentation reports available from NTIS or at no charge or nominal cost from Agricultural Research Service; (2) Familiarization may take several man-weeks due to the lack of detailed documentation reports; (3) Data preparation and actual computational costs are unknown

Table 3A-9. Summary of ACTMO (continued)

Characteristic	Summary Data
Model Accuracy and Sensitivity	(1) Mass balance for chemicals considers transport via both runoff and erosion (sediment-attached); (2) Simulation of watershed zones (and tubes) permits consideration of a wide variety of crops and systems topography; (3) Model application for flat terrain difficult due to requirements for gravity-induced cascading between zones; (4) ACTMO only permits evaluation of one chemical type and one application per simulation run
Other Comments	(1) Salt movement and salinity are not considered in ACTMO; (2) Chemical model requires only one crop type per zone; (2) Model originators: (a) ACTMO developed by U.S. Dept. of Agriculture, Agricultural Research Service personnel, (b) USDAHL-74 is revised program based on USDA Hydrograph Lab--1970 model from ARS, Beltsville, Md.

Table 3A-10. Summary of Storage, Treatment, Overflow and Runoff Model (STORM)

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Urban; (2) General nonurban
Time Properties	(1) Continuous simulation with hourly time step; (2) Input hourly precipitation and daily air temperature; (3) Output hourly, event, and/or annual summaries; (4) Run for extended periods, usually a year or more
Space Properties	Small to large single catchment
Physical Properties	(1) Rainfall/snowmelt runoff estimated by runoff coefficient method or Soil Conservation Service method; (2) Dry-weather flow quantity estimated by coefficient method, daily and hourly variation factors included; (3) Wet-weather quality estimated using linear residuals buildup with washoff rate proportional to runoff; (4) Erosion estimated by Universal Soil Loss equation, no interaction of "erosion" with other residuals, (5) Dry-weather quality estimated by coefficient method, (6) No treatment is assumed to occur in storage; (7) Treatment is simply a hydraulic accounting of flow-through capability, no explicit removal of residuals
Chemical Processes	(1) Quality constituents represented as conservative substances; (2) Suspended and settleable solids, BOD, total nitrogen, and orthophosphate are represented
Ecological Processes	Coliforms.are represented
Economic Analysis	None
Mathematical Properties	Deterministic model with iterative solution of algebraic equations
Computational Status	(1) Coded in Fortran IV; (2) Operational on IBM 360 series, CDC 6600, and UNIVAC 1108; (3) Storage requirements: 50,000 words of core storage; (4) Input by card reader and/or tape/disk
Input Data Requirements	(1) Hourly precipitation and daily air temperature; (2) Land use including runoff parameters; (3) Residuals accumulation and washoff rates; (4) Land surface erosion parameters; (5) Treatment rate and storage volume
Ease of Application	(1) Nonproprietary model; (2) Updated user's manual available from Hydrologic Engineering Center (HEC), U.S. Army Corps of Engineers, Davis, California; (3) Documentation includes hardware and software requirements, brief subroutine description, data input specifications, default data, and test problems; (4) User support is available through HEC; (5) Used extensively in EPA 208 and other studies throughout the U.S.
Output and Output Format	(1) Four types of output: quantity analysis, quality analysis, pollutograph analysis, land surface erosion analysis; (2) Quantity and quality reports include annual statistics of rainfall/snowmelt runoff, residuals washoff, and the quantity, quality, and frequency of overflows; (3) Land surface erosion report shows average annual values for sediment production and delivery
Linkages to Other Models	(1) Linked to SWMM - RECEIV by Meta Systems; (2) Linked to simplified SWMM RECEIVE by Medina
Manpower Needs	(1) Environmental engineer; (2) Systems programmer
Costs	(1) Model available at nominal cost (about $50) from HEC; (2) Precipitation and air temperature data tapes available from U.S. Weather Service for about $100; (3) Land use data usually available at little cost; (4) One year simulation costs about $1.00
Model Accuracy and Sensitivity	(1) STORM is used as a preliminary model to provide rough estimates of runoff quantity and quality, and required sizes of storage and treatment; (2) Neglecting the treatment in storage may mislead user into specifying two separate control units when a single storage/treatment unit could be used
Other Comments	(1) A very popular model that has undergone extensive testing and refinement; (2) Excellent user support available

Table 3A-11. Summary of the Quantity-Quality-Simulation Model (QQS)

Characteristic	Summary Data
Applicable Land Drainage Area	Urban
Time Properties	(1) Continuous (up to 2,000,000 time steps) or single event simulation using a 5-minute time step; (2) Input precipitation data: (a) at 5-minute intervals for continuous simulation and for single event simulation, (b) output at time step intervals for selected events plus event, annual, and total summaries and statistics; (3) up to a 20-year simulation.
Space Properties	(1) Small to medium multiple catchments; (2) Discretization limits: (a) surface: lumped simulation of inlet hydrograph for up to 100 subcatchments and three input hyetographs, (b) channel/pipes: one-dimensional simulation, limit of 400 sewer network elements, 35 overflow points, 15 basins or pumps, 20 operational controls, recommended maximum element length = 500 m
Physical Processes	(1) Surface quantity: conversion of rainfall to inlet hydrographs by unit hydrographs for routing of rainfall excess, recovery of depression storage between storms; (2) Channel/pipes and receiving waters: flow routing by kinematic wave and equations for special structures (e.g., weirs), storage routing, backwater effect, surcharging, looped connection, pressure flow simulated by alternate solution of equation in downstream, then upstream direction at each time step; (3) Dry-weather flow quantity and quality on basis of diurnal variation and population density; (4) Surface quality washoff by empirical formula, a function of dust/dirt loadings and number of time steps from beginning of storm, street sweeping simulated; (5) Quality routing through channel/pipes, storage units and receiving water by plug flow, no scour or deposition, removal by treatment element a function of flow rate
Chemical Processes	Generation and routing of up to four arbitrary conservative residuals, empirical surface washoff functions available for BOD, COD, suspended solids, settlable solids, total nitrogen, total PO_4, fecal coliform
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	(1) Deterministic model; (2) Surface quantity: unit hydrograph calculations, separate for pervious and impervious areas; (3) Channel/pipes and receiving waters: implicit finite difference solution to simplified St. Venant equations; (4) Surface quality, quality routing and treatment: algebraic equations, no iterations required once flows and velocities are known
Computational Status	(1) Coded in Fortran IV, approximately 30,000 statements, requires 122 K (UNIVAC); (2) Has been run on UNIVAC 1108 and 1110, DEC 2050, Amdahl 470
Input Data Requirements	(1) Historical or synthetic rainfall record: at 5-minute time intervals, evaporation rates; (2) Surface quantity: area, imperviousness, unit hydrographs for pervious and impervious areas, depression storage, infiltration rates; (3) Surface quality: maximum dust/dirt accumulation rates, pollution buildup and washoff functions, street sweeping interval and efficiency, land use; (4) Water use, population density, diurnal dry-weather flow quantity/quality variation; (5) Channel/pipes and receiving waters: linkages, shape, length, slope, roughness, parameters for other elements (e.g., weirs, pumps, storages, time and water depth dependent operational controls); (6) No input data required for channel/pipe and receiving water quality routing; (7) Treatment parameters for removal as function of flow rate in treatment and storage elements; (8) Large reduction in data requirements possible by aggregating (lumping) of subcatchments and channel/pipes, especially useful for continuous simulation; (9) All data may be in metric or U.S. customary units
Ease of Application	(1) Nonproprietary model available from EPA, Edison, N.J.; (2) User's manual and thorough documentation published as EPA reports; (3) Test cases documented in EPA report; (4) Initial model setup often moderately difficult due to size
Output and Output Format	(1) Input data summary including precipitation; (2) Hydrographs and pollutographs (concentrations and loads versus time) at any point in system on time step, no stages or velocities printed; (3) Total flow volumes and quality loads for events and longer intervals; (4) Annual and monthly frequencies and durations for overflow volumes, hydrograph and pollutograph peaks, volumes, concentrations, loads, removal in storage/treatment units, etc., frequency-duration curves tabulated and plotted on line printer; (5) Other summary statistics and frequency distributions; (6) Monthly, annual, and total summaries for continuous simulations; (7) All output in either metric or U.S. customary units (corresponding to choice for input data), column headings in English
Linkages to Other Models	None (simple receiving water routing included)
Manpower Needs	(1) Environmental engineer with knowledge of urban hydrological processes for data reduction and model analysis; (2) Systems programmer for model setup

Table 3A-11. Summary of QQS Model (Continued)

Characteristic	Summary Data
Costs	(1) Model available upon receipt of cost of magnetic tape from EPA (2) Data assembly and preparation may require multiple man-weeks for a large catchment or urban area; (3) Computer costs moderately high for simulation of 20-year record on urban area using aggregation of subcatchments and channel/pipes; (4) Quality calculations will be subject to extensive calibration if accuracy is desired for single event or continuous simulation; quantity calibration is relatively simple
Model Accuracy and Sensitivity	(1) Quantity simulation may be made quite accurate with relatively little calibration; (2) Quality simulation requires more extensive calibration using measured residuals concentrations, quality results might be inaccurate without calibration on local measurements; (3) Hydraulic computations adequate for systems without and with surcharging, pressure flow, or extensive backwater; (4) Sensitivity to input parameters depends upon given system configuration; (5) Quality results most sensitive to assumed surface dust/dirt loadings
Other Comments	QQS is more detailed than most continuous simulation models and is thus useful for detecting flooding/backwater problems in the system as well; (2) The extensive statistical output provides more information than most continuous models; (3) The model has been applied at several European and North American cities

Table 3A-17. Summary of the Agricultural Runoff Model (AGRUN)

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Agriculture: (a) crops, (b) pasture
Time Properties	(1) Single runoff event simulation; (2) Inputs: precipitation data at 15 minute intervals, daily data for other parameters; (3) Outputs: simulation of time history results based on 15 minute intervals
Space Properties	(1) Small to large multiple catchments; (2) Dimensionality: (a) multiple dimensions: two-dimensional land surface, three-dimensional subsurface layers, one-dimensional stream channel; (3) Discretization limits: (a) watershed may be divided into as many as 200 subareas, (b) subareas may vary in size, (c) tributary drainage system may have up to 200 channels in dendritic pattern (lengths and cross sections can vary), (d) can handle up to 5 soil layers
Physical Processes	(1) Overland flow across land surface and in small stream channels; (2) Groundwater interflow; (3) Channelized tributary flow; (4) Sediment erosion estimated with Universal Soil Loss Equation
Chemical Processes	(1) Constituent transport limited to sediment-attached parameters; (2) All constituents considered conservative--no interaction or degradation; (3) Constituents represented: total suspended solids, BOD, and fecal coliforms are operational
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	Using numerical integration of differential equation set
Computational Status	(1) Coded in Fortran IV; (2) Requires IBM 360/365 digital computer or equivalent; (3) Computer core storage requirements unspecified, but extensive
Input Data Requirements	(1) Precipitation data and drainage channel specifications; (2) Land use hydrogeometric data; (3) Watershed and soil characteristics
Ease of Application	(1) Nonproprietary model derived from SWMM Runoff Module; (2) Basic SWMM documentation available from NTIS or EPA Planning Assistance Branch, Washington, D.C.; (3) Documentation report from Iowa-Cedar River Basin Project available from Water Resources Engineers, Walnut Creek, Ca. or EPA Systems Development Branch, Washington, D.C.; (4) Extent of documentation: (a) SWMM documentation fairly complete for most applications, (b) AGRUN report presents brief information on model modifications, data deck design, sample input and output formats, but no program listings
Output and Output Format	(1) Print of model inputs; (2) Rainfall hyetograph (rate vs. time history) by catchment; (3) Time history of runoff in user-specified stream channels; (4) Time history of sediment concentration in user-specified stream channels, (5) Time history of constituent concentration in stream channels
Linkages to Other Models	(1) Designed to link with nonsteady state receiving water models; (2) Hydrologic linkages result from tributary channel inputs and groundwater inputs (interflow); (3) Final tributary channel output serves as input to receiving water model
Manpower Needs	(1) Environmental engineer experienced in water resources and water quality modeling; (2) Familiarity with Storm Water Management Model and its application useful
Costs	(1) Model acquisition costs are unknown; (2) Program listings could probably be obtained from WRE--Walnut Creek or EPA Planning Assistance Branch for a nominal reproduction charge; (3) Data preparation costs: actual computational costs are unknown
Model Accuracy and Sensitivity	(1) AGRUN can closely simulate watershed with numerous different fields and crop types; (2) Constituent transport limited to sediment-adsorbed substances; (3) No constituent interactions permitted--assumption probably valid if residence time in channels short; (4) No quality constituent (dissolved) transport permitted in groundwater interflow; (5) Rainfall intensity assumed to be uniform over each subcatchment
Other Comments	(1) Only sediment-attached residuals can be simulated; (2) Model originators: (a) AGRUN is a derivative of SWMM for nonurban applications, (b) AGRUN was developed by Water Resources Engineers, Walnut Creek, Ca. for EPA Systems Development Branch, Washington, D.C.

Table 3A-13. Summary of the SOGREAH CAREDAS Model

Characteristic	Summary Data
Applicable Land Drainage Area	Urban
Time Properties	(1) Single precipitation events with unsteady flows; (2) Input and output at arbitrary time intervals, time step adjustment during program execution to minimize computer time, no upper limit on number of time steps
Space Properties	Small to medium multiple catchments; unlimited number of catchments, pipes, special structures, overflow points.
Physical Processes	(1) Surface: conversion of rainfall to inlet hydrographs by: (a) unit hydrograph, (b) empirical French Caquot method (similar to unit hydrograph), or (c) user supplied methodology, surface routing by Muskingum method is optional, dry-weather flow as hydrographs; (2) Channel/pipe network: flow routing through dendritic, branching, or looped network including effects of backwater, flow reversal, and surcharging, modeled network facilities include pumps, siphons, weirs, flap valves, and internal storage; (3) Routing of up to 10 conservative or first-order nonconservative water quality constituents via advective-diffusion equation in channel/pipe network, user must supply inlet pollutographs (concentration-time curves), no sedimentation in storage elements
Chemical Processes	None other than routing through channel/pipe system
Ecological Processes	None
Economic Analysis	None
Mathematical Properties	(1) Deterministic model with implicit finite-difference solution of de St. Venant equations for channel/pipe flow routing; (2) Explicit finite-difference solution of advective-diffusion equation for water quality constituent routing (3) Channel/pipe routing in branched, steep portions of network can be performed optionally using Cunge-Muskingum method.
Computational Status	Coded in Fortran IV for IBM equipment; dynamic storage, memory needs depend on size of simulated system
Input Data Requirements	(1) Historical or synthetic hyetograph at arbitrary time intervals; (2) Surface: area, imperviousness, slope, length, runoff coefficient or Horton infiltration coefficients, Muskingum routing coefficients; (3) Channel/pipes: (a) linkages, length, shape, roughness, invert and ground elevations; (b) geometric and hydraulic parameters describing other elements such as weirs, pumps, siphons, valves, and storages; (4) First-order decay coefficients for quality constituents; (5) All data are metric
Ease of Application	(1) Proprietary model for use through SOGREAH, New York, N.Y.; (2) User's manual available; (3) May be run in modular form
Output and Output Format	(1) Input data summary; (2) Output stages, velocities, hydrographs and pollutographs (concentration-time) at arbitrary time invervals and locations, plotting options; (3) All output in metric, French, German and English column headings available
Linkages to Other Models	(1) Linked to SOGREAH receiving water model; (2) User may supply own routines for generation of inlet hydrographs and must supply own routine for generation of inlet pollutographs
Manpower Needs	(1) Environmental engineer with knowledge of urban hydrological and hydraulic process; (2) Systems programmer for support
Model Accuracy and Sensitivity	(1) Surface: unit hydrographs and empirical formulations will require moderate calibration efforts; (2) Channel/pipes: solves complete dynamic St. Venant equations providing high accuracy simulation of complex hydraulic phenomena, e.g., backwater, flow reversal, surcharging, pressure flow; (3) Implicit numerical integration technique helps avoid stability problems; (4) Sensitivity to input parameters depends upon given system configuration; (5) Cunge-Muskingum option simulates fewer hydraulic phenomena, but allows rapid, inexpensive preliminary design.
Other Comments	(1) The strength of CAREDAS is in the highly sophisticated channel/pipe hydraulic routines, quality routines are relatively weaker; (2) CAREDAS has been applied to several European and African cities. North American offices of SOGREAH are in New York City and Lasalle, Quebec

Table 11-14. Summary of EPA Storm Water Management Model (SWMM) Including Water Resources Engineers (WRE) Transport Model

Characteristic	Summary Data
Applicable Land Drainage Area	(1) Urban; (2) General nonurban
Time Properties	(1) Single event or continuous simulation, latter has unlimited number of time steps, former usually limited to 150-200 but can be unlimited also, depending on portions of model utilized, continuous version simulates only surface runoff (including simple gutter/pipe routing) and storage/treatment: (2) Precipitation: input at arbitrary time intervals for single event simulation (typically 1-15 min.) and at one-hour intervals for continuous simulation, for snowmelt simulation daily max-min temperatures required for continuous, time step temperatures for single event; (3) output at time step intervals (or multiples), daily, monthly, annual, and total summaries for continuous simulation; (4) Time step arbitrary for single event (typically 5 minutes) and one hour for continuous, WRE transport model time step depends on stability criteria, may be as small as a few seconds
Space Properties	(1) Small to large multiple catchments: (a) surface: lumped simulation of overland flow with allowance for up to 200 subcatchments and six input hyetographs, up to 200 gutter/pipes may be simulated by one-dimensional routing, (b) channel/pipes: one-dimensional network, up to 159 conduit/nonconduit elements for original transport model, up to 239 conduits in WRE transport model, up to two in-line storage units in original transport model, (c) catchment area may be disaggregated and modeled sequentially for simulation of areas too large for existing SWMM dimensions, (d) storage/treatment simulated separately, receiving input from upsteam routing, (e) output from surface, channel/pipe, or storage/treatment simulation may serve as new input for further simulation by the latter two modules
Physical Processes	(1) Flow derived from precipitation and/or snowmelt; snow accumulation and melt simulated using temperature-index methods developed by National Weather Service, snow redistribution (e.g., plowing, removal) may be simulated; (2) Overland flow by nonlinear reservoir using Manning's equation and continuity, depression storage, Green-Ampt or integrated Horton infiltration, recovery of depression storage via evaporation between storms during continuous simulation, also exponential recovery of infiltration capacity; (3) Channel/pipes: (a) nonlinear reservoir formulation for gutter/pipes in surface runoff portion of SWMM, includes translation and attenuation effects, (b) kinematic wave formulation in original transport model assumes cascade of conduits, cannot simulate backwater over more that one conduit length, surcharging handled by storing water at surcharged junction pending available flow capacity, (c) WRE transport model solves complete St. Venant equations including effects of backwater, flow reversal, surcharging, looped connection, pressure flow, (d) infiltration and dry-weather flow may enter conduits of original and WRE transport simulation; (4) Storage routing using modified Puls method assuming horizontal water surface, outlets include pumps, weirs, orifices; (5) Surface quality on basis of linear buildup of dust/dirt during dry-weather and associated residuals fractions, exponential washoff with decay parameter a function of runoff rate, erosion by Universal Soil Loss Equation; (6) Dry-weather flow quantity and quality on basis of diurnal and daily variation, population density and other demographic parameters, buildup of suspended solids in conduits by dry-weather deposition using Shield's criterion; (7) Quality routing by advection and mixing in conduits and by plug flow or complete mixing in storage units, scour and deposition of suspended solids in conduits (original transport model) using Shield's criterion; (8) Storage/sedimentation residuals removal as exponential function of residence time; (9) Treatment devices include swirl concentrator, micro strainer, dissolved air flotation, biological, removal based on empirical equations, usually a function of flow rate
Chemical Processes	(1) Eight conservative residuals (BOD, suspended solids, settleable solids, COD, total nitrogen, total PO_4, oil/grease, total coliforms), plus one user-supplied, plus erosion simulated in surface runoff portion; (2) BOD, SS, coliforms routed through remainder of model; (3) BOD subject to first order decay during routing using decay coefficient = 0.2 day^{-1}
Ecological Processes	(1) Coliform washoff is included; (2) Biological treatment is simulated
Economic Analysis	Amortized capital plus operation and maintenance costs for control units are determined
Mathematical Properties	(1) Deterministic model; (2) Surface quantity: iterative solution of coupled continuity and Manning equations, integrated form of Horton infiltration (infiltration rate proportional to cumulative infiltration, not time), or Green-Ampt; (3) Surface gutter/pipe routing; nonlinear reservoir assuming water surface parallel to invert; (4) Channel/pipes: (a) original transport: implicit finite difference solution to modified kinematic wave equation, (b) WRE transport: explicit finite difference solution of complete St. Venant equations, stability may require short time step; (5) Storage/sedimentation: modified Puls method requires table look-up for calculation of outflow; (6) Surface quality, quality routing and treatment: algebraic equations, no iterations required once flows and conduit volumes are known
Computational Status	(1) Coded in Fortran IV, approximately 25,000 statements long; (2) Has been run on IBM 360 series, UNIVAC 1108, CDC 6600, Amdahl 470 and others; may be run in modular form (surface runoff, original or WRE transport, storage/treatment, receiving water, plus executive and service routines, e.g., plotting, file combining), largest module requires about 90,000 words or 360K bytes of storage; (3) Available on a magnetic tape; (4) Requires up to five off-line storage files

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Table 3A-14. Summary of EPA SWMM Including WRE Transport (continued)

Characteristic	Summary Data
Input Data Requirements	(1) Historical or synthetic precipitation record, uses National Weather Service precipitation tapes for continuous simulation, monthly evaporation rates for snowmelt: daily max-min (continuous) or time-step (single event) temperatures, monthly wind speeds, melt coefficients and base melt temperatures, snow redistribution fractions and areal depletion curves (continuous only), other melt parameters; (2) Surface quantity: area, imperviousness, slope, width, depression storage and Manning's roughness for pervious and impervious areas, infiltration parameters; (3) Channel/pipe quantity: linkages, shape, slope, length, Manning's roughness, WRE transport also requires invert and ground elevation, storage volumes at manholes and other structures, geometric and hydraulic parameters for weirs, pumps, orifices, storages, etc., infiltration rate; (4) Storage/sedimentation quantity: geometry, hydraulic characteristics of outflows; (5) Surface quality: land use, total gutter length, catchbasin volume and initial residuals concentrations, street sweeping interval, efficiency and availability factor, dry days prior to initial precipitation, dust/dirt and residuals fraction parameters for each land use if Chicago default values are not used, or user-supplied initial residuals surface loadings, exponential washoff coefficient, erosion parameters for Universal Soil Loss Equation, if simulated; (6) Dry-weather flow on basis of diurnal and daily quantity/quality variations; population density, other demographic parameters; (7) No input data required for channel/pipe quality routing; (8) Storage/treatment: parameters defining exponential removal as function of residence time in storage/sedimentation, parameters for individual treatment options, e.g., particle size distribution, maximum flow rates, size of unit, chemical additions, optional dry-weather flow data when using continuous simulation; (9) Storage/treatment costs: ENR index, unit costs of excavation, land, power, chlorine, polymers, alum, interest rate and amortization period; (10) Data requirements for individual modules much less than for run of whole model, large reduction in data requirements possible by aggregating (lumping) of subcatchments and channel/pipes, especially useful for continous simulation
Ease of Application	(1) Nonproprietary model available from EPA, Washington, D.C. or University of Florida, Department of Environmental Engineering Sciences, Gainesville; (2) Updated user's manual and thorough documentation of most routines published as EPA reports, no one report covers all model aspects; (3) Test cases documented in several EPA and other reports; (4) Short course proceedings also useful for model applications; (5) U.S. and Canadian user groups with newsletters and semi-annual meetings permit publication of changes; (6) Due to its age (originally published in 1971), availability, documentation, examples of SWMM usage are widely available in the literature; (7) Frequent model update/corrections/improvements are often difficult to learn about, new model released approximately on an annual basis; (8) Size of model most frequent deterrent to use, however, see item 10 above under Input Data Requirements; (9) Initial model setup often moderately difficult due to size
Output and Output Format	(1) Input data summary including precipitation; (2) Hydrographs and pollutographs (concentrations and loads versus time) at any point in system on time step or longer basis, no stages or velocities printed; (3) WRE transport also outputs elevation of hydraulic grade line; (4) Surcharge volumes and required flow capacity, original transport model will resize conduits to pass required flow (optional); (5) Removal in storage/treatment units, generated sludge quantities; (6) Summaries of volumes and residuals loads for simulation period, continuity check, initial and final pounds of solids in conduit elements: (7) Daily (optional), monthly, annual and total summaries for continuous simulation, plus ranking of 50 highest hourly precipitation, runoff and BOD values; (8) Line printer plots of hyetographs, hydrographs, and pollutographs; (9) Costs of simulated storage/treatment options
Linkages to Other Models	(1) SWMM contains its own receiving water model, RECEIV; (2) Individual modules and the total SWMM model have been linked to the HEC STORM model, the QUAL-II model, simplified receiving water models, and others; (3) Individual modules (e.g., surface runoff, receiving water) have been altered and renamed by various groups
Manpower Needs	(1) Environmental engineer familiar with urban hydrological processes for data reduction and model analysis; (2) Systems programmer for model setup and off-line storage file usage
Costs	(1) Model available upon receipt of cost of magnetic tape plus a nominal charge (about $40 from University of Florida) or no other charge (from EPA); (2) Data assembly and preparation may require multiple man-weeks for a large catchment or urban area; (3) Example computer execution costs given in user's manual, on the order of $20 for a surface runoff and transport run for a single storm event with about 50 subcatchments and channel/pipes, use of WRE transport can be more costly due to short time step, continuous simulation of one subcatchment with snowmelt for two years costs about $20; (4) Extensive calibration may be required to duplicate measured quality results, quantity calibration relatively simple; (5) National Weather Service precipitation tapes for continuous simulation cost about $100 for a 25-year hourly record
Model Accuracy and Sensitivity	(1) Quantity simulation may be made quite accurate with relatively little calibration; (2) Quality simulation requires more extensive calibration using measured residuals concentrations, quality results will almost certainly be very inaccurate without local measurements; (3) WRE transport accurately simulates backwater, flow reversal, surcharging, pressure flow, original transport routines may be used at less cost if these conditions not present; (4) Sensitivity to input parameters depends upon schematization, however, surface quality predictions are most sensitive to dust/dirt and residuals fraction loading rates

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Table 3A-14. Summary of EPA SWMM Including WRE Transport (continued)

Characteristic	Summary Data
Other Comments	(1) SWMM is perhaps the most widely used urban runoff/quality model because of its early development, availability and documentation, its major weakness is its sheer size, several portions of the model have been adapted for use in other models; (2) Several comparative studies have been made of SWMM and other models, permitting evaluation by potential users; (3) Use of SWMM for continuous simulation is relatively untested and more expensive than use of the HEC STORM model. SWMM's main advantage is a superior storage/treatment routine, which accounts for treatment that occurs in storage, although STORM will do this also in the future; other potential SWMM advantages include flow routing and snowmelt procedures; disadvantages include difficulty of determining proper Horton infiltration parameters on natural or agricultural areas and weaker statistical summaries; (4) The WRE transport model is the most sophisticated channel/pipe flow routing model available in the public domain; (5) Original model developers: Metcalf and Eddy, Palo Alto, Ca, Water Resources Engineers, Walnut Creek, Ca., and University of Florida, Department of Environmental Engineering Sciences, Gainesville, Fl.; EPA has supported continued maintenance and updating by the last developer since 1971, moderate user support is also available

Appendix B. ANNOTATED REFERENCES FOR MODEL SUMMARY TABLES

Brandstetter, A. B. 1976. Assessment of Mathematical Models for Storm and Combined Sewer Management, Report No. EPA-600/2-76-175a, prepared for Environmental Protection Agency, Cincinnati, Ohio, August and available as NTIS Publication No. PB-259-597.

This is the best single reference for a tabulation, summary, and comparison of all major urban runoff models.

Brown, J. W., M. R. Walsh, R. W. McCarley, A. J. Green, and H. W. West. 1974. Models and Methods Applicable to Corps of Engineers Urban Studies, Misc. Paper H-74-8 (Vicksburg, Mississippi, Waterways Experiment Station, U.S. Army Corps of Engineers, August) and available as NTIS Publication No. AD-786-516.

This contains very useful, standardized summaries of many urban, nonurban, and receiving water models. It provides much information not easily obtainable elsewhere.

Chow, V. T. and B. C. Yen. 1976. Urban Stormwater Runoff: Determination of Volumes and Flowrates, Report No. EPA-600/2-76-116, prepared for Environmental Protection Agency, Cincinnati, Ohio, May, and available as NTIS Publication No. PB-253-410.

This includes a discussion of eight urban runoff models/techniques.

Chu, C. S. and C. E. Bowers. 1977. Computer Programs in Water Resources, WRRC Bulletin 97 (Minneapolis, Minn., Water Resources Research Center, University of Minnesota, November).

This is a summary of characteristics of twenty-eight hydrologic models, including some test results and an annotated bibliography.

Colyer, P. J. and R. W. Pethick. 1976. Storm Drainage Design Methods, A Literature Review, Report No. INT 154 (Wellington, Oxfordshire, England, Hydraulics Research Station, March).

This contains a good summary of urban drainage technique as well as computer models.

Environmental Protection Agency. 1976. Areawide Assessment Procedures Manual, Appendix A, Model Applicability Summary, Report No. EPA-600/9-76-014 (Cincinnati, Ohio, July).

This reference indentifies and discusses eight runoff models considered operational: STORM, SWMM, HSP, MITCAT, HVM-QQS, simplified SWMM, AGRUN, and ILLUDAS. Good evaluations are provided.

Fleming, G. 1975. Computer Simulation Techniques in Hydrology (New York, American Elsevier).

This contains capsule summaries of many hydrologic models (no quality), as well as an extensive discussion of the Stanford Model.

Grimsrud, G. P., E. J. Finnemore, and H. J. Owen. 1976. *Evaluation of Water Quality Models: A Management Guide for Planners*, Report No. EPA-600/5-76-004, prepared for Environmental Protection Agency, Athens, Ga., July.

This publication deals primarily with receiving water models and only peripherally with runoff models.

Heeps, D. P. and R. G. Mein. 1973. *An Independent Evaluation of Three Urban Stormwater Models*, Civil Engineering Research Report No. 4/1974 (Victoria, Australia, Monash University).

__________ and __________. 1974. "Independent Comparison of Three Urban Runoff Models," *Journal of Hydraulics Division, Proceedings of the American Society of Civil Engineers* vol. 100, no. HY7 (July) pp. 995-1009.

These two references give a comparative evaluation of the SWMM, RRL, and UCUR models.

Huber, W. C. 1975. "Modeling for Storm Water Strategies," *APWA Reporter* vol. 42, no. 5 (May) pp. 10-14.

This includes a somewhat dated table of characteristics of fifteen urban runoff models plus discussions of SWMM and STORM.

__________, J. P. Heaney, and H. C. Torno. 1977. "Computer Impact on Environmental Runoff and Wastewater Studies," Preprint No. 3106. Paper presented at the American Society of Civil Engineers Fall Convention, San Francisco, Calif., October 17-21.

This contains a useful discussion of modeling caveats as well as a good bibliography related to widely-used models.

James F. MacLaren, Ltd. 1975. *Review of Canadian Design Practice and Comparison of Urban Hydrologic Models*, Research Report No. 26, prepared for Canada-Ontario Research Program, Environmental Protection Service, Environment Canada, Ottawa, Ontario, October.

Included are detailed comparative tests of the SWMM, RRL, UCUR, HVM, and MITCAT models as well as the rational method.

Lager, J. A., W. G. Smith, W. G. Lynard, R. M. Finn, and E. J. Finnemore. 1977. *Urban Stormwater Management and Technology Update and User's Guide*, Report No. EPA-600/8-77-014, prepared for Environmental Protection Agency, Cincinnati, Ohio, September and available as NTIS Publication No. PB-275-654.

This includes tables of urban runoff model characteristics and good examples of the use of screening (Level I) models.

Lumb, A. M. 1976. *Comparison of the Georgia Tech, Kansas, Kentucky, Stanford, and TVA Watershed Models in Georgia*, Report ERC-0476 (Atlanta, Ga., Environmental Resources Center, Georgia Institute of Technology, January).

This contains a useful taxonomy of Stanford Watershed Model variants as well as model comparisons.

Marsalek, J., T. M. Dick, P. E. Wisner, and W. G. Clarke. 1975. "Comparative Evaluation of Three Urban Runoff Models," *Water Resources Bulletin* vol. 11, no. 2 (April) pp. 306-328.

This contains comparisons of the SWMM, RRL, and UCUR models.

McPherson, M. B. 1975. *Urban Hydrological and Catchment Research in the U.S.A.*, Technical Memo No. IHP-1 (New York, American Society of Civil Engineers Urban Water Resources Program, November) and available as NTIS Publication No. PB-260-685.

This publication is especially useful for relating urban runoff models to locations where they have been applied.

Ott, W. R., ed. 1976. *Proceedings of the EPA Conference on Environmental Modeling and Simulation*, Report No. EPA-600/9-76-016 (Cincinnati, Ohio, Environmental Protection Agency) and available as NTIS Publication No. PB-257-142.

The background and application of many different runoff models are illustrated in various papers within these proceedings.

Overton, D. E. and M. E. Meadows. 1976. *Stormwater Modeling* (New York, Academic Press).

This includes a good discussion of kinematic wave technique and models used in the TVA region.

Papadakis, C. N. and H. C. Preul. 1973. "Testing of Methods for Determination of Urban Runoff," *Journal of Hydraulics Division, Proceedings of the American Society of Civil Engineers* vol. 99, no. HY9 (September) pp. 1319-1335.

This contains a comparison of the UCUR, SWMM, RRL, and Chicago Hydrograph models.

Proctor and Redfern, Ltd. and James F. MacLaren, Ltd. 1976a. *Storm Water Management Model Study, Vol. I: Final Report*, Research Report No. 47 prepared for Canada-Ontario Research Program, Environmental Protection Service, Environment Canada, Ottawa, Ontario, September.

Proctor and Redfern, Ltd. and James F. MacLaren, Ltd. 1976b. *Storm Water Management Model Study, Vol. II: Technical Background*, Research Report No. 48, prepared for Canada-Ontario Research Program, Environmental Protection Service, Environment Canada, Ottawa, Ontario, September.

Although centered around the SWMM model, useful tables are included characterizing other models, and requirements for modeling cold weather conditions are given in these two reports.

U.S. Forest Service. 1977. *Non-Point Water Quality Modeling in Wildland Management: A State-of-the-Art Assessment*, Report No. EPA-600/3-77-036, prepared for Environmental Protection Agency, Athens, Ga., April.

This has perhaps the best current summary of nonurban runoff models.

Viessman, W., Jr., J. W. Knapp, G. L. Lewis, and T. E. Harbaugh. 1977. *Introduction to Hydrology*, 2nd ed. (New York, Intext Educational Publishers).

In addition to explanations of hydrologic analysis techniques, this excellent text has brief descriptions of several widely-used models, including a discussion of water quality.

Wanielista, M. P. 1978. *Stormwater Management, Quantity and Quality* (Ann Arbor, Mich., Ann Arbor Science Publishers).

Several modeling techniques for urban and rural areas are discussed.

ACTMO

Frere, M. H., C. A. Onstad, and H. N. Holtan. 1975. *ACTMO--An Agricultural Chemical Transport Model*, Publication No. ARS-H-3 (Hyattsville, Md., Agricultural Research Service, U.S. Department of Agriculture).

Holtan, H. N., G. N. Stiltner, W. H. Henson, and H. C. Lopez. 1975. *USDAHL-74 Revised Model of Watershed Hydrology*, Technical Bulletin No. 1518 (Washington, D.C., Agricultural Research Service, U.S. Department of Agriculture, December).

AGRUN

Roesner, L. A., S. W. Zison, J. R. Monser, and T. C. Lyons. 1975. *Agricultural Watershed Runoff Model for the Iowa-Cedar River Basins*, prepared for the Environmental Protection Agency, Systems Development Branch, Washington, D.C. by Water Resources Engineers, Walnut Creek, Calif.

ARM

Donigian, A. D., Jr., D. C. Beyerlein, H. H. Davis, and N. H. Crawford. 1977. Agricultural Runoff Management (ARM) Model--Version II: Refinement and Testing, Report No. EPA-600/3-77-098, prepared for Environmental Protection Agency, Athens, Ga., August.

CAREDAS

SOGREAH. 1973. "Mathematical Flow Simulation Model for Urban Sewerage Systems, CAREDAS Program," partial draft. Translated by D. Vetrano (Richland, Wash., Battelle-Northwest, December).

__________. 1977. Mathematical Model of Flow in an Urban Drainage Programme, SOGREAH Brochure 06-77-33-05-A (Grenoble, France, SOGREAH).

EPARRB

True, H. A. 1976a. "Planning Models for Non-Point Runoff Assessment," in W. R. Ott, ed., Proceedings of the Conference on Environmental Modeling and Simulation, Report No. EPA-600/9-76-016 (Cincinnati, Ohio, Environmental Protection Agency, July) pp. 74-76 and available as NTIS Publication No. PB-257-142.

__________. 1976b. "Non-Point Assessment Processes." Draft (Athens, Ga., Environmental Protection Agency).

HSP

Hydrocomp, Inc. 1976. Hydrocomp Simulation Programming and Operations Manual 4th ed. (Palo Alto, Calif., Hydrocomp, Inc.).

__________. 1977. Hydrocomp Water Quality Operations Manual (Palo Alto, Calif., Hydrocomp, Inc.).

Hydroscience Simplified Model

Environmental Protection Agency. 1976. Areawide Assessment Procedures Manual, Volumes I-III, Report No. EPA-600/9-76-014 (Cincinnati, Ohio, July et seq.).

MRI

McElroy, A. D., S. Y. Chiu, J. W. Nebgen, A. Aleti, and F. W. Bennett. 1976. Loading Functions for Assessment of Water Pollution from Nonpoint Sources, Report No. EPA-600/76-151, prepared for Environmental Protection Agency, Washington, D.C., May, and available as NTIS Publication No. PB-253-325.

NPS

Donigian, A. S., Jr. and N. H. Crawford. 1976. Modeling Nonpoint Pollution from the Land Surface, Report No. EPA-600/3-76-083, prepared for Environmental Protection Agency, Athens, Ga., July, and available as NTIS Publication No. PB-250-566.

__________ and __________. 1977. Simulation of Nutrient Loadings in Surface Runoff with the NPS Model, Report No. EPA-600/3-77-065, prepared for the Environmental Protection Agency, Athens, Ga., June.

QQS

Geiger, W. F. 1977. "Continuous Unsteady Simulation with QQS (Concept-Program-Tests-Application)," paper presented at the EPA SWMM Users' Group Meeting, Gainesville, Fla., April 4-5.

__________. 1975. "Urban Runoff Pollution Derived from Long-Term Simulation," in Proceedings of National Symposium on Urban Hydrology and Sediment Control (Lexington, Ky., University of Kentucky, July) pp. 259-270.

__________, S. A. LaBella, and G. C. McDonald. 1976. "Overflow Abatement Alternatives Selected by Combining Continuous and Single Event Simulations," in Proceedings of National Symposium on Urban Hydrology and Sediment Control (Lexington, Ky., University of Kentucky, July) pp. 1-9.

__________ and H. R. Dorsch. 1980. Quantity-Quality Simulation (QQS) - A Detailed Continuous Planning Model for Urban Runoff Control, Volume I -- Model Description, Verification, and Applications. Report No. EPA-600/ , prepared for Environmental Protection Agency, Cincinnati, Ohio.

__________ and __________. 1980. Quantity-Quality Simulation (QQS) - A Detailed Continuous Planning Model for Urban Runoff Control, Volume II -- User's Manual, Report No. EPA-600/ , prepared for Environmental Protection Agency, Cincinnati, Ohio.

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Lager, J. A., T. Didriksson, and G. B. Otte. 1976. Development and Application of a Simplified Stormwater Management Model, Report No. EPA-600/2-76-218, prepared for Environmental Protection Agency, Cincinnati, Ohio, August, and available as NTIS Publication No. PB-258-074.

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Chapter Four

ANALYZING SURFACE RECEIVING WATER BODIES

Melvin O. Hinson, Jr., and Daniel J. Basta

INTRODUCTION

Surface receiving water systems[1] are defined as surface water bodies into which residuals are directly or indirectly discharged. Surface receiving water systems include: flowing and intermittent streams, rivers, lakes, ponds, reservoirs, estuaries, and offshore marine systems. The last systems consist of waters which generally lie outside salinity transition zones but receive residuals via tidal exchange, ocean outfalls, and dumping, e.g., barge or dredge discharges. Boundaries for analyzing a given receiving water system will vary depending on the management context. For example, a receiving water system under study may be comprised of an entire river basin including lakes, tributaries, and mainstream segments, or be limited to only certain river segments. For a riverine system, upstream boundaries are likely to be defined by first-order tributaries and downstream boundaries by the junction with a larger river channel or at the salinity transition zone in an estuary. Natural boundaries for an estuarine or marine system are defined by shorelines, the junctions with inflowing streams, and somewhat arbitrary seaward boundaries, the last often set at the end of the salinity transition zone. However, the boundaries for analyzing a given estuarine system are likely to consist of the estuarine system plus all of the major tributaries.

This chapter provides background and information for the selection of natural systems models (NSMs) for receiving water systems for use in analysis for REQM in various REQM contexts. The chapter is organized in four sections.

The first section identifies and describes briefly the major ambient water quality problems associated with receiving waters. In all REQM contexts, at least one of the problems identified is likely to be of concern. The recognition of these problems over time has stimulated the development and refinement of NSMs for assessing the effects of alternative physical measures for improving ambient water quality. Hence, some discussion of the types of problems is warranted, including those for which no accurate operational NSMs existed at the end of 1978.

The second section identifies and describes briefly the natural processes--physical, chemical, biological--which operate in receiving water bodies. These processes affect the movement and transformation of residuals in receiving water bodies, movement and transformations which result in the problems identified in the previous section. It follows that in order to estimate the temporal and spatial patterns of ambient water quality resulting from residuals discharges, the relevant processes must somehow be taken into account. The extent and manner in which a receiving water model incorporates the relevant processes and the empirical data available to verify the model determine how accurately the model represents the real world.

The third section describes the basic approaches used to formulate receiving water models. This section builds upon the related section in chapter 2, by describing how the general analytical approaches explained in chapter 2 are modified for application to receiving water bodies.

The fourth section indicates how to select, for any given REOM context, one or more receiving water NSMs from a set of existing operational models. This section is directly related to the section in chapter 2 on setting up the analysis of natural systems. Four major elements comprise this section: (1) a listing of a large number of receiving water models, both operational and nonoperational, referred to as the population table; (2) a table which relates receiving water problem characteristics to operational NSMs, referred to as the problem table; (3) a flow diagram which shows the procedure for selecting a receiving water NSM given the material in the chapter, referred to as the selection procedure; and (4) a discussion of the characteristics used to summarize operational receiving water NSMs.

Appendix A contains detailed summary tables for 27 operational receiving water NSMs. Appendix B contains a list of annotated references for each of the 27 operational NSMs summarized, and references, not annotated, for models in the population table which are not considered to be operational as of the end of 1978.

MAJOR AMBIENT QUALITY PROBLEMS ASSOCIATED WITH RECEIVING WATERS

When residuals discharges into a receiving water body exceed its natural assimilative capacity, myriad problems can result: decreased propagation of fish and wildlife; transmission of disease to humans; reduced aesthetic properties; and reduced utility of water for beneficial uses other than fish and wildlife. However, many of these problems are also the results of naturally occurring processes which are accelerated by man's activities, not solely the results of residuals discharges. Major water quality problems are: temperature, salinity, sedimentation, dissolved oxygen, eutrophication, toxic substances, and biological effects. Whatever the questions posited regarding ambient water quality in a given REQM context, one or more of these problems will be involved.

Temperature

Temperature is a measure of the ambient thermal condition of a receiving water body, as measured on a definite scale, e.g., degrees Fahrenheit, degrees Celsius, degrees Kelvin (absolute). Temperature in a receiving water body is a function of such variables as: solar heat inputs; hydrodynamic properties of the water body, e.g., mixing characteristics, flow conditions, water body depth; and other external heat inputs, e.g., geothermal springs, residual heat from electrical energy generation and industrial processes. Aside from the obvious effects on changes of state, e.g., freezing and evaporation, the level of temperature and temperature changes have various impacts on receiving water bodies. Temperature affects the viscosity of water, which in turn affects flow characteristics, and affects water density, which in turn affects thermal stratification.[2] Temperature also has impacts on: physicochemical reactions, e.g., dissolved oxygen saturation and reaction rates: biochemical reactions, e.g., bacterial decomposition; biological processes, e.g., photosynthesis and respiration; and on the behavioral patterns of organisms, e.g., initiation of feeding and spawning.

Heat discharges from man's activities can alter natural temperature conditions in receiving waters, with possible adverse effects on resident aquatic organisms. Resident organisms acclimated to seasonal patterns of thermal conditions are stressed by higher than average temperatures and related changes in reaction rates of many processes as a result of residual heat discharges. Depending on the organism, the level of temperature, and the magnitude of change in thermal conditions, permanent injury or mortality can result. Heat discharges can also result in synergistic effects, e.g., the adverse effects of low dissolved oxygen concentration are exacerbated by higher temperature. For a discussion of the effects of heat and temperature on living organisms in receiving waters see section III in National Academy of Sciences (1972).

Salinity

Salinity problems are associated with high concentrations of total dissolved solids, consisting mainly of inorganic salts and a small amount of organic material. Salinity can be a major problem not only because of its effects on organisms within receiving water bodies, but also because of its effects on uses of water withdrawn from receiving water bodies. Uses affected include water for drinking, for irrigation of crops, and for industrial activities.

Salinity problems in freshwater systems result from the fact that resident flora and fauna communities lack appropriate physiological mechanisms to counter the osmotic stresses of high dissolved solids concentrations. However, in estuarine systems where dynamic transitions in salinity occur, i.e., fresh to brackish to saline, resident organisms usually have physiological mechanisms which enable them to minimize osmotic stresses due to rapid changes in salinity, over some range. Salinity is rarely a quality problem in most coastal marine systems, except where discharges of highly concentrated brines occur and when large outflows of freshwater, as in large floods, reduce salinity substantially below normal.

Salinity in receiving waters is a greater problem in arid and semi-arid regions, such as the irrigated areas of the western United States, where high evaporation and low precipitation rates result in concentration of salts in surface waters and in the uppermost layers of the soil profile. These accumulated salts can become a water quality problem when precipitation or applied irrigation water redissolves them and runoff carries them into local receiving waters, or when they are leached into groundwater and subsequently discharged to receiving water. Natural sources of saline discharges, such as salt springs, and runoff from saline soils, constitute significant nonpoint sources.

Sedimentation

Erosion is the naturally occurring geologic process involving the removal of soil and rock particles from the land surface and their transport to receiving water bodies. Over time this process has been accelerated in many areas by the removal of natural vegetative cover by man's activities. The types of material and the ways in which they are transported to receiving water bodies after being dislodged are referred to as the sediment transport process in chapter 3 (p. 141).

Once the sediment has reached a receiving water body, it is subject to two basic processes, transport and sedimentation. Sediment carried in suspension in moving water is termed suspended sediment or suspended solids.[3] Sediment which remains in contact with the bed as it moves is termed bed load. Total sediment load is the sum of the two. Sedimentation is the process by which sediment settles or deposits, under the force of gravity, on the bottom of a receiving water body, e.g., stream, lake, estuary. Sediment which has settled may be resuspended as a result of flood flows, tidal action, or passage of vessels.

Suspended solids in flowing water can adversely affect many uses of water and many aquatic organisms. High suspended solids concentrations diminish light penetration and inhibit photosynthesis by aquatic organisms. Sediment deposited on stream beds, river beds, and on the bottoms of lakes can smother bottom dwelling plants and organisms and fish spawning grounds. Sediment entering receiving waters can also carry attached nutrients, pesticides, and heavy metals, all of which in themselves have various effects on ambient water quality. Other problems attributed to sediment in receiving waters include clogging of filters at water treatment plants, filling in of navigation channels, and reduction of reservoir capacities. However, not all the effects of sediment in streams are adverse. In some cases suspended solids concentrations have been sufficiently high to preclude significant algae growth and hence reduce taste and odor problems in municipal water supplies.

Not all sediment in receiving water bodies is a result of discharges into receiving water bodies. Flowing water can generate sediment by eroding stream banks and stream beds. Therefore, instream suspended solids concentrations and bed loads may or may not be reduced by decreasing sediment discharges into receiving streams. Because flowing streams and rivers have a certain amount of potential energy--depending on flow and gradient--reducing sediment inputs releases the energy which would be used to carry the sediment, thereby potentially increasing the erosive impacts of the stream with respect to its banks and bed. If the stream channel consists of easily erodible material, such as alluvium, the stream will erode, scour, and gouge its course until it is again carrying sediment at its carrying capacity. That capacity may, of course, be altered by the process, because of a change in gradient, resulting in a new equilibrium. Vanoni (1976) provides a detailed technical discussion of sediment transport and deposition. Sediment problems in general are discussed in Stall (1972) and Wade and Heady (1978).

Dissolved Oxygen

Dissolved oxygen is a water quality indicator which is a measure of the concentration of oxygen in a receiving water body. Dissolved oxygen is important because a substantial amount of dissolved oxygen must be maintained in a receiving water body in order for many organisms to survive and to sustain aerobic decomposition of organic matter and oxidation of chemical compounds. Oxygen enters a receiving water body across the air-water interface in response to an oxygen deficit, which is the difference between the ambient concentration of dissolved oxygen and the prevailing oxygen saturation level. The amount of oxygen which will dissolve in water, entering across the interface, depends primarily on percent saturation of the receiving water body, water temperature, and atmospheric conditions of temperature and pressure. Such factors as the presence of thermal or salinity stratifications, flow conditions as they affect turbulence, benthic (bottom) deposits of organic matter, and light penetration also affect dissolved oxygen concentration.

The primary demand for oxygen in a receiving water body is a result of the demand for oxygen to decompose organic material discharged into the water body. Three indicators are used in relation to the oxygen demand of a water body: biochemical oxygen demand (BOD); chemical oxygen demand (COD); and total organic carbon (TOC). BOD is a measure of the total amount of of a change in gradient, resulting in a new equilibrium. Vanoni (1976) provides a detailed technical discussion of sediment transport and deposition. Sediment problems in general are discussed in Stall (1972) and Wade and Heady (1978).

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Over the years, dissolved oxygen has been used as a general indicator of the health of a water body. However, evidence in recent years has shown that dissolved oxygen alone is an inadequate indicator of the overall health of a water body and that other indicators are also required. Nevertheless, dissolved oxygen remains an important indicator of the ability of a water body to sustain life and to assimilate residuals. A low level of dissolved oxygen in a receiving water body is very likely to indicate the existence of a major problem.

Eutrophication

Eutrophication is the normally slow aging process by which a lake evolves into a bog or marsh and ultimately is entirely filled in. There are two interrelated components of this process. The first is the gradual accumulation of sediment and debris in the lake which, over time, decreases depth. The second is the effect on plant growth within a lake of nutrients which enter a lake in solution, attached to soil particles, or both. The growth of aquatic plants is the principal focus of the eutrophication problem. During eutrophication, a lake becomes so rich in nutrient compounds that algae and other plant life grow in abundance until they literally begin to choke the lake. This phenomenon can eventually result in "drying up" the lake. In most cases, the principal nutrients affecting eutrophication are nitrogen (N) and phosphorus (P). However, other factors having a strong influence on plant growth include: currents within a lake which move nutrients into, within, and out of the system; changes in dissolved oxygen concentrations in lower levels of a lake that affect decomposition processes which in turn release nutrients; and the amount of light penetration.

Usually the effects of eutrophication are undesirable. Aesthetic and recreational values of receiving water bodies decrease because of floating algae and undesirable odors produced by eutrophication. When water supplies are drawn from receiving water bodies undergoing eutrophication, algae hinder treatment plant operations, e.g., clogging filters and often causing undesirable tastes and odors. In a few situations the effects of eutrophication can be positive, at least for some period of time as, for example, when the increase in amount of plant life in a water body results in increased fish production.

Human activities have accelerated eutrophication in many water bodies in the United States. Nitrogen, phosphorus, and other nutrients are discharged into receiving waters from such sources as municipal wastewater treatment plants, industrial operations, crop growing agricultural operations, animal feedlots, and runoff from both urban and nonurban areas. At the same time, the demand for the recreational services of water bodies has intensified. Eutrophication has been recognized as a sufficiently important ambient water quality problem to prompt the initiation of the National

Eutrophication Survey, which is carried out each year.[4] Among the references which include discussions of eutrophication are Middlebrooks, Falkenborg, and Maloney (1974), and Allen and Kramer (1972). An excellent compilation of references was contained in Eutrophication: A Bimonthly Summary of Current Literature, published by the Water Information Program at the University of Wisconsin at Madison.

Toxic Substances

A toxic substance is one which, on coming into contact with an organism--fish, animal, human--will over time cause some degree of morbidity or mortality. Much controversy exists as to the evidence required to establish whether or not a compound is a toxic substance.[5] Given that there were approximately 60,000 chemicals in common use in the United States in 1978, with many being added each year, the overwhelming magnitude and complexity of the toxic substances problem becomes clear.

The toxic substances problem with respect to receiving waters involves analyzing the movement, transformation, and effects of such substances discharged into receiving waters. Little is known about the behavior and temporal effects of most chemical compounds discharged into receiving waters. Toxic effects on plant and animal life in receiving waters have been found to result from discharges of: (1) herbicides, insecticides, rodenticides, and other pesticides; (2) heavy metals such as lead, zinc, mercury; (3) radioactive materials, which are generally toxic both because of radioactivity and because of the heavy metal form of the material; (4) oils, both refined and crude; (5) reduced ions such as ammonia, cyanides, and sulfides; and (6) miscellaneous hydrocarbons, such as chloroform, aromatics, and phenols.

Biological Effects

Biological effects relate to the impacts of residuals discharges on resident aquatic organisms or on terrestrial animals which directly utilize receiving water bodies.[6] Thus, this problem is closely related to all of the problems mentioned previously. Depending on the context, some estimate of the impacts on living organisms of levels and variations in temperature, salinity, sedimentation, dissolved oxygen concentration, eutrophication, and the amounts and types of discharges of toxic substances, will almost always be desired, whether or not the biological effects can be rigorously quantified. Hence, biological effects are not "a problem" in the same sense as the other problems. But they are identified as a problem because of the way in which questions to be answered in an REQM analysis are often posed. Frequently the problem is stated in terms of why some observed biological effect occurred. For example, a problem may be defined as the reduction in the production of a certain fish species in a particular receiving water body. The reason for the decrease in fish production may be the result of one or more of the major problems mention, or of other problems, but the problem has not been perceived in those terms. The symptom is perceived rather than the cause. Thus, identifying biological effects as a problem is useful for organizing an analysis of ambient water quality problems and their related impacts.

Types of biological effects include: transmission of pathogenic bacteria and viruses to man or other terrestrial animals via direct contact or drinking of water; chronic toxicity effects, such as decreased population sizes; increased metabolic stresses on organisms; decreased productivity of autotrophic organisms;[7] and changes in competition, feeding, and reproductive patterns. Because biological populations respond both dynamically and simultaneously with one another to changes in ambient water quality, it is often difficult to identify the impacts of a residual on specific members of an aquatic community. Because effects on biological populations are often the result of cumulative responses to multiple factors, segregating responses to an individual residual from responses to normal variations in the ambient quality of receiving water bodies is difficult.

Summary Comments

The potential problems described in this section represent the major water quality problems in receiving waters which are likely to be encountered in analyses for REQM. However, no claim is made that all water quality problems of receiving waters can be grouped under these headings. Nevertheless, these seven problems provide an operational basis for identifying the capabilities of the operational receiving water NSMs summarized in Appendix A. The seven are used as the major headings in the problem table which relates operational NSMs to problems in the section on selecting an appropriate receiving water NSM. For many specific problems within each major problem category, either no NSMs currently exist, or those that do exist are still in the developmental stage as the end of 1978.

MAJOR NATURAL PROCESSES

In a receiving water body, numerous natural processes are at work. These processes affect the movement of water, the related transport of materials and energy by water, and the transformations of both material and energy that take place in the receiving water body. These processes, in conjunction with discharges of residuals from man's activities and inputs of material and energy as a result of natural processes,[8] result in the problems described in the previous section. Materials, including residuals, which are not transformed chemically while being transported in receiving water bodies are termed conservative substances. Those which are transformed during transport are termed nonconservative substances. An example of a material usually assumed to be a conservative substance is dissolved salts, which do not react chemically or biochemically to any significant degree with other materials in receiving waters.[9] Examples of nonconservative substances are biodegradable organic matter and the reduced ionic states of nitrogen. These undergo chemical, physicochemical, and biochemical reactions in receiving waters. Heat, as an energy residual discharged from man's activities, is also nonconservative.

Five types of natural processes--discussed below--occur in receiving water bodies: (1) physical processes, also termed hydraulic or physical transport processes; (2) chemical processes; (3) physicochemical processes; (4) biochemical processes; and (5) ecological processes. The extent to which different NSMs explicitly take these processes into account varies substantially. For example, purely statistical NSMs entail no explicit consideration of these processes. Thus it is important to understand the natural phenomena involved in order to select an appropriate NSM for a given context and to interpret results after the NSM has been applied.

Physical (Hydraulic) Transport Processes

The movement of water is the primary mechanism which transports material and energy into, within, and out of a receiving water body. Physical (hydraulic) transport processes bring about: (1) the movement of water through a receiving water body; and (2) the movement of material and energy within the water moving through the receiving water body.

The amount of water moving through a receiving water body at any given time is a function of the net amount of water entering the system, and of the physical characteristics and geometry of the water body, including slope, depth, channel and tributary configuration, composition of strata, and man-made diversions or barriers to flow, for example, dams, channels, bridge abutments and dredged channels. This description is an oversimplification and clearly does not pertain exactly to all receiving water bodies. For example, in estuaries, water movement is also affected by tidal action. In shallow coastal marine systems, such as bays, water movement may be the result solely of wind action, or solely of temperature (convection), or of both. Nevertheless, the description does indicate the basic factors which condition water movement.

The net amount of water entering a receiving water body is a function of two factors: one, the hydrologic cycle, and two, residuals discharges from man's activities. The hydrologic cycle is defined as the circuit of water movement from the atmosphere to the earth and return to the atmosphere. This cycle involves various processes: precipitation, interception, runoff, infiltration, percolation, storage, evaporation, and transpiration (Betts, et al., 1962).[10] The hydrologic cycle was discussed in chapter 3.

Depending on the water body and related conditions, the movement of material and energy within the water moving through a receiving water body is primarily a function of three physical processes: advection, diffusion, and convection. Advection and diffusion were defined and discussed in chapter 2. Convection is the movement of water, and the material or energy contained in the water, caused by differences in density due to nonuniform temperature and the force of gravity. The net effect of convection is to produce a diffusion type transport of materials or energy in a water body. Convection is an important process to consider in various combinations of problem contexts and water bodies. One example was indicated above regarding water movement in shallow coastal water bodies. Another example is the case where discharges of thermal residuals are a major factor. Convection is also important in impoundments where water moves through the system very slowly and temperature differences between portions of the water body affect water movement, e.g., temperature differences between warm, shallow water near shore and colder, deeper water farther from shore.

Note that diffusion is identified above as one process. This is not really the case. As indicated in chapter 2, there are several types of diffusion including: Brownian motion of molecules, eddy diffusion due to the swirling motion of a fluid, and diffusion via turbulent mixing due to the random motion of microscopic particles. Another diffusion type process important in receiving water systems is hydrodynamic dispersion. Hydrodynamic dispersion occurs when residuals located in the boundary layer of flowing water move more slowly than residuals located farther from the boundaries. The motion of the residuals located in the boundary layer is retarded, inducing a spreading or "apparent diffusion" in the direction of the flow, termed longitudinal dispersion. See figure 3-13, and Daily and Harleman (1966) and Fischer (1967, 1973) for additional discussion.

Because it is often impossible to distinguish among the various types of diffusion type processes in the real world, most receiving water models lump all types of diffusion into a single diffusion coefficient, which incorporates the net effect of all diffusion type processes. The value of the coefficient will vary depending on which diffusion process or processes is or are dominant in a water body under given conditions. Therefore, throughout the remainder of this chapter, reference will be made only to the diffusion process and not to individual diffusion processes.

The distinction made between physical (hydraulic) processes which affect the movement of water through a water body and physical (hydraulic) processes which affect the movement of material and energy within the water moving through the water body is important, because the conservation of mass and energy approach to analyzing receiving water bodies subdivides the analysis into these two parts.

Chemical and Physicochemical Processes

The physical (hydraulic) transport processes discussed above account for the movement of both conservative and nonconservative substances in receiving waters. However, these processes have little or no effect on the transformations of nonconservative substances which take place in receiving water. These transformations are caused by reactions which are the result of chemical, physicochemical, and biochemical processes. (Biochemical processes are discussed in the following section.)

Chemical processes involve the reaction of two or more compounds with each other to form one or more different compounds. The principal chemical processes affecting chemical reactions in water bodies are oxidation-reduction processes and ionic dissociation. A chemical compound is oxidized when it loses one or more electrons to another compound. The compound receiving electrons in the transfer is said to be reduced. Both compounds are transformed as a result of the reaction. Many of the most important chemical reactions (transformations) which take place in water bodies are the result of oxidation-reduction processes. Ionic dissociation is the process whereby a substance separates (dissociates) into a simpler form without a transfer of electrons taking place. An example is the dissociation of acetic acid in water, i.e., $HC_2H_3O_2$ dissociates into H + $C_2H_3O_2$. (The reverse process of association also takes place in water bodies.) Both processes affect the transformation of organic and inorganic nonconservative substances, as they are transported in water bodies. The processes of oxidation-reduction and ionic dissociation in water bodies are discussed in Sienko and Plane (1961) and in Morris (1956).

Physicochemical processes involve both the chemistry and physics of molecules as they interact in their surroundings. Principal physicochemical processes affecting either the transformation of substances or the movement of substances in water bodies are: adsorption-desorption, absorption, and gravity settling. Adsorption is the adhesion of a substance to the surface of a solid or liquid. Adsorption is an important process because many residuals, such as nitrogen and phosphorus compounds, pesticides, heavy metals, attach themselves to soil particles and are transported through receiving water bodies with the soil particles. Desorption is the reverse process, by which a substance is detached from the surface of a solid or liquid. For example, adsorbed residuals which have been deposited on the bottom of a water body with the material to which they have adhered, can become detached when disturbed by dredging, tidal action, or scouring by flood waters.

Absorption is the penetration of one substance into or through another substance. Perhaps the most important manifestation of the absorption process is the absorption of oxygen from the atmosphere at the air-water interface. This is the primary mechanism through which receiving water bodies obtain dissolved oxygen. Gravity settling is the process of deposition under the force of gravity, usually on the bottom of a water body. Such settling can concentrate residuals in bottom sediments and can adversely affect benthic organisms.

The rates at which these chemical, physicochemical and biochemical reactions occur is important in understanding ambient water quality. Because many of the reactions of interest proceed so slowly, the rate of reaction is of major importance. The rate of reaction is dependent on the individual material and the extent to which interactions with other materials take place. The study of the time pattern of reaction rates and of the conditions which affect those rates is known as chemical reaction kinetics. In chemical reaction kinetics, reactions are classified as zero-order, first-order, second-order, or third-order processes, as illustrated in table 4-1.

Table 4-1. Classification of Chemical Reaction Kinetics

Order of Process	Rate Term	Apparent Reaction
zero	k	M_1 products
first	kc_1	M_1 products
second	$kc_1{}^2$	$M_1 + M_1$ products
second	kc_1c_2	$M_1 + M_2$ products
third	kc_2c_3	$M_1 + M_2 + M_3$ products
third	$kc_1{}^2c_2$	$M_1 + M_1 + M_2$ products
third	$kc_1{}^3$	$M_1 + M_1 + M_1$ products

Note: k is a constant of proportionality and c_1, c_2, and c_3 are concentrations of the materials M_1, M_2, and M_3 respectively. Rates are given as mas per unit volume per time interval, for example, mg. per ccm. per second.

A zero-order process means that the rate at which a certain material changes into another form of the same material is constant and not dependent upon the concentration in the receiving water body of that material or any other materials. A zero-order process for an inorganic chemical transformation is defined by the equation $\frac{dc}{dt} = k$, where k = constant and c = amount of reactant. A first-order process, where the rate of change is proportional to the amount of material present, is defined by $\frac{dc}{dt} = kc$, where k = constant and c = amount of material available for reaction. In a second-order process, material interacts with itself or other materials in producing the final products. Similarly, a third-order process implies that the rate of change is dependent on various combinations of three interacting substances. Although second- and third-order processes are characteristic of many complex inorganic chemical reactions, most receiving water NSMs utilize only first-order kinetics to describe such reactions as dissolved oxygen reaeration, ammonium oxidation, and BOD oxidation.

Biochemical Processes

A biochemical process is a process in which a chemical reaction takes place as a result of living organisms in the biological cycle. Two phases exist in the biological cycle, regardless of whether the system under scrutiny be on land or in any of the numerous different types of receiving waters. These two phases are growth and decay, both of which are always simultaneously occurring in natural systems. For example, during the growth phase, plant growth in a water body increases and energy from sunlight is stored in the biomass. During the decay phase, the reverse takes place, i.e., biomass decreases and energy is released. In receiving water bodies, the two most important processes of growth and decay are photosynthesis and bacterial decomposition, respectively.

Photosynthesis is the principal way in which solar energy is converted by living organisms. In this process, carbon dioxide and water are converted into carbohydrates and oxygen in green plants. In water bodies, photosynthesis produces dissolved oxygen and organic matter, e.g., algae, bottom plants. The biomass created also absorbs materials such as phosphorus, nitrogen compounds, metals such as cadmium, magnesium, silica, and other minor nutrients. Photosynthesis is an important process in water quality analyses because: (1) it is the primary natural process which effects eutrophication; and (2) the various substances which biomass absorbs have significant effects on the kinetics of many chemical reactions in receiving waters.

Bacterial decomposition is the oxidation of organic material by bacteria and other lower forms of life. This process consumes oxygen, reduces biomass or organic matter to a lower form, and in so doing releases stored chemical energy in the products of decomposition, e.g., carbon dioxide, nitrogen. The utilization of oxygen in this way is known as respiration. Bacterial decomposition is the so-called basic self-cleaning process in a water body. When water bodies are anaerobic, i.e., have an oxygen deficiency, it is the result of bacterial decomposition requiring more oxygen for the oxidation of organic material than is available in the water body. Hence, this process is a major oxygen depletion mechanism which must be considered in NSMs.

Photosynthesis and bacterial decomposition are balancing, closely related processes. The oxygen produced during photosynthesis is used during bacterial decomposition, and the products of decomposition are used during photosynthesis to build biomass. Many ambient water quality problems are the result of a stability state reached between these two processes, which state is incompatible with man's intended use of a given water body.

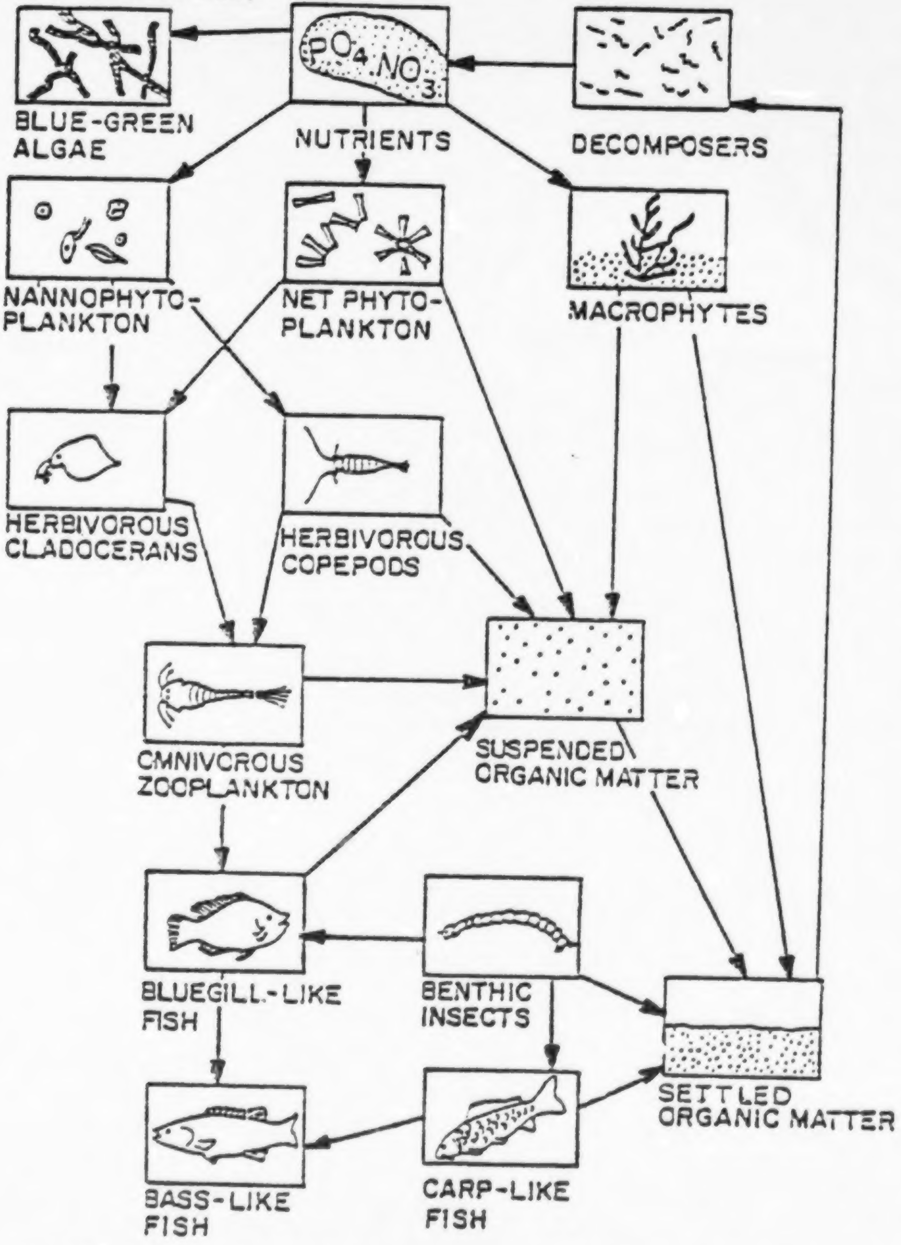
It should be emphasized that biochemical reactions are extremely complicated and generally not well understood. This stems from the complexity of the molecules involved and the many pathways through living organisms which affect the reactions. Phelps (1953) provides an excellent discussion of these processes in relation to water quality.

Ecological Processes

Ecological processes are very closely related to biochemical processes. However, whereas biochemical processes such as photosynthesis and bacterial decomposition involve direct linkages to substances in water, ecological processes relate to direct linkages among different species of living organisms.

Ecological linkages involve the consumption of one species or organism by another which is higher in the food chain, and the consumption of that species by another, and so on. The food chain begins with the production of organic material by photosynthesis, termed primary production in ecological nomenclature. This material is consumed by "grazing organisms" which in turn are consumed by other higher organisms. Grazing organisms are categorized as the first trophic level; the organisms or animals which feed upon them are categorized as the second trophic level; animals which feed on organisms or animals in the second trophic level are categorized as the third trophic level; and so on. Organisms or animals which are on the same trophic level are the same number of steps removed from primary production in a receiving water body. Figure 4-1 illustrates typical

Figure 4-1. Illustration of Typical Ecological Linkages in Receiving Water Body


BLUE-GREEN ALGAE
PO4 NO3
NUTRIENTS
DECOMPOSERS
NANNOPHYTO-PLANKTON
NET PHYTO-PLANKTON
MACROPHYTES
HERBIVOROUS CLADOCERANS
HERBIVOROUS COPEPODS
OMNIVOROUS ZOOPLANKTON
SUSPENDED ORGANIC MATTER
BLUEGILL-LIKE FISH
BENTHIC INSECTS
SETTLED ORGANIC MATTER
BASS-LIKE FISH
CARP-LIKE FISH

Source: Modified from figure 1 in Clifford S. Russell, editor, Ecological Modeling in a Resource Management Framework, Proceedings of a Symposium by National Oceanic and Atmospheric Administration and Resources for the Future (Washington, D.C., Resources for the Future, 1975) p. 55.

ecological linkages in a receiving water, in this case a lake.

The number of organisms in each trophic category in a receiving water body will vary with time and in space due to processes such as growth, respiration, mortality (both natural and due to predation by other organisms), movement across system boundaries, and intrasystem movements due to currents or tidal action. Depending on the organism, the movement of water wihin a water body will have more or less effect on the movement of the organism. For example, the movement of planktonic algae depends entirely on water movements, and therefore the algae can be assumed to be transported in water just as are conservative chemical substances. On the other hand, free-swimming organisms--from microscopic zooplankton to fish--can move under their own "power," and hence are less affected by currents within receiving waters.

The analysis of ecological processes is extremely difficult. Analyzing the processes involved, such as respiration and growth, usually involves consideration of second- and third-order kinetics. The complexity of the mathematical functions necessary to describe these higher order kinetics requires data which often far exceed the amount and quality of data available. Even so, ecological processes are extremely important and merit explicit consideration, because many of man's uses of water bodies relate directly to the organisms and animals which reside in the water.

Summary Comments

It is difficult to conceptualize how all these processes interrelate and occur simultaneously in a receiving water body. The foregoing descriptions of the major processes are brief. Nevertheless, understanding these processes--the actual physical phenomena which affect water quality--is crucial in order to select one or more NSMs which will be appropriate in a given context.

For each operational receiving water NSM summarized in Appendix A, information relating to how these processes are considered is indicated in the summary tables. For purposes of compactness, the five processes discussed above are aggregated into three categories on the model summary tables: physical; chemical, which includes physicochemical, chemical, and biochemical; and ecological. Some additional discussion of these processes is contained in the section on selecting an appropriate receiving water NSM.

APPROACHES TO ANALYZING RECEIVING WATER SYSTEMS

Chapter 2 identified and described the two basic approaches for analyzing natural systems, conservation of mass and energy and statistical. This section briefly describes how these approaches are applied to the analysis of receiving water bodies. It should be emphasized that the material presented in this section is not a substitute for the more detailed texts and reports available on analyzing different types of receiving water bodies. Rather, this section--intended as an overview--should complement the many available references on the subject, some of which are identified below.

Conservation of Mass and Energy Approach for Analyzing Receiving Water Bodies

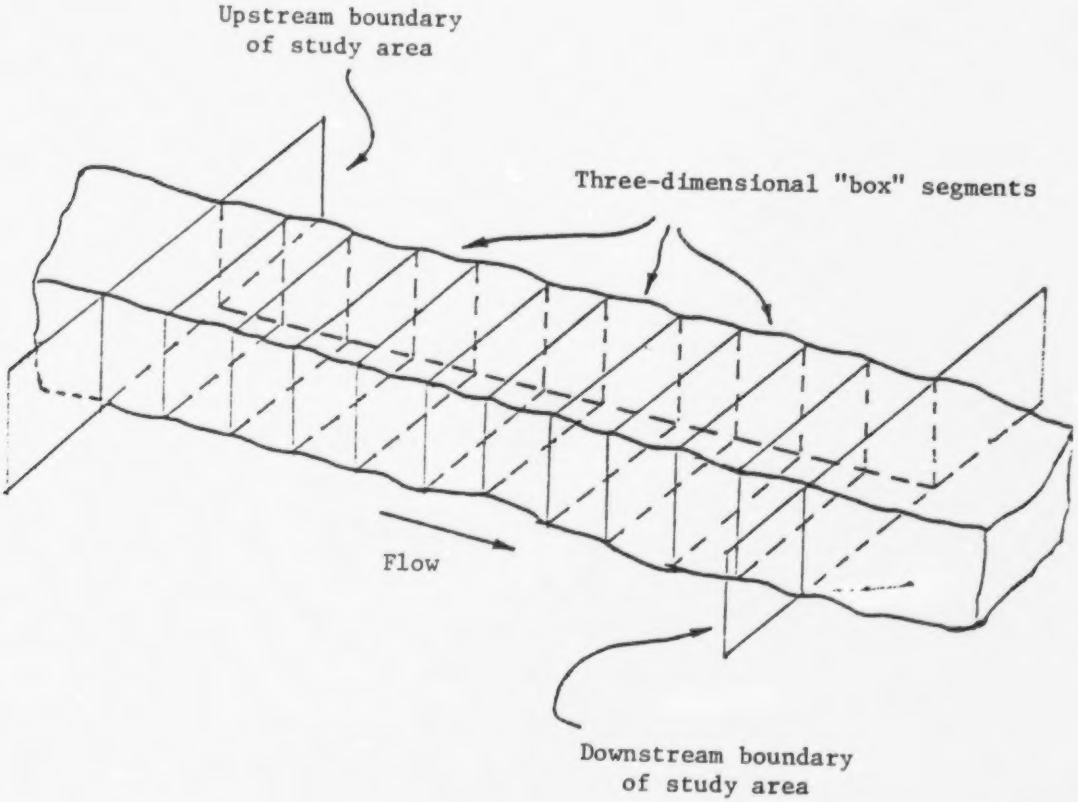
The conservation of mass and energy approach has been widely used for many years to analyze receiving water bodies. During this time, many and varied models using this approach have been developed. The model form depends on the type of water body, flow conditions, the problem context, and the assumptions made. The degree of complexity varies from simple mass balances to complex sets of simultaneous differential equations.

The conservation of mass and energy approach, as applied to receiving water bodies, is comprised of four "building blocks" regardless of the type of water body or flow conditions. These are: the hydraulic block, the physical transport block, the chemical reaction block, and the ecological block. Depending on the question(s) to be addressed, two or more of the blocks are used. The essence of the conservation of mass and energy approach is to account for the movement of mass, of energy, or of both into and out of each volume into which a receiving water body may be divided.

In order to explain these building blocks, visualize a simple three-dimensional box. Consider this three-dimensional box as one of the volumes into which a receiving water body is divided, as illustrated in figure 4-2. The first building block relates to estimating the quantity of water which enters and exits the box within a given time period. Often referred to as the hydraulic portion of a receiving water NSM, the analysis involves mathematically representing the relevant hydraulic processes and estimating the velocities at which water moves through parts of the water body, based on the geometry and other physical characteristics of the water body and the energy gradient. In many operational receiving water NSMs, this first building block is implicit rather than explicit. That is, the hydraulic inputs are obtained exogenously to the model.[11]

The second building block relates to estimating the quantity of material which is transported into and out of the box within the water. This involves representing mathematically the physical processes which govern the movements of material in water, i.e., advection and diffusion. (These

Figure 4-2. Three-Dimensional Segmentation of a River


Upstream boundary of study area
Three-dimensional "box" segments
Flow
Downstream boundary of study area

are referred to in the section on physical transport processes and discussed in chapter 2.) In order to calculate the quantity of material entering and exiting the box, hydraulic information from building block 1 becomes input into building block 2.

If, in a given problem context, the residuals of concern are conservative materials, e.g., total dissolved salts or suspended solids, then the NSM applied in the REQM analysis would only have to be comprised of building blocks 1 and 2--hydraulic and physical transport respectively--assuming that the NSM satisfied all other requirements such as required accuracy and available resources. However, if the residuals of concern are not conservative materials, e.g., organic materials, then a third building block would have to be added.

The third building block relates to estimating changes in the quantities of nonconservative materials and energy which take place within the box. This involves representing mathematically the chemical reactions--including biochemical and physicochemical--and specifying the appropriate reaction kinetics which affect these transformations. It follows that in order to estimate the amount of nonconservative substance entering or exiting the box in a given time period, or the ambient concentration of a nonconservative AEQ indicator within the box, the equations developed in building block 3 must be combined with those of building blocks 1 and 2.

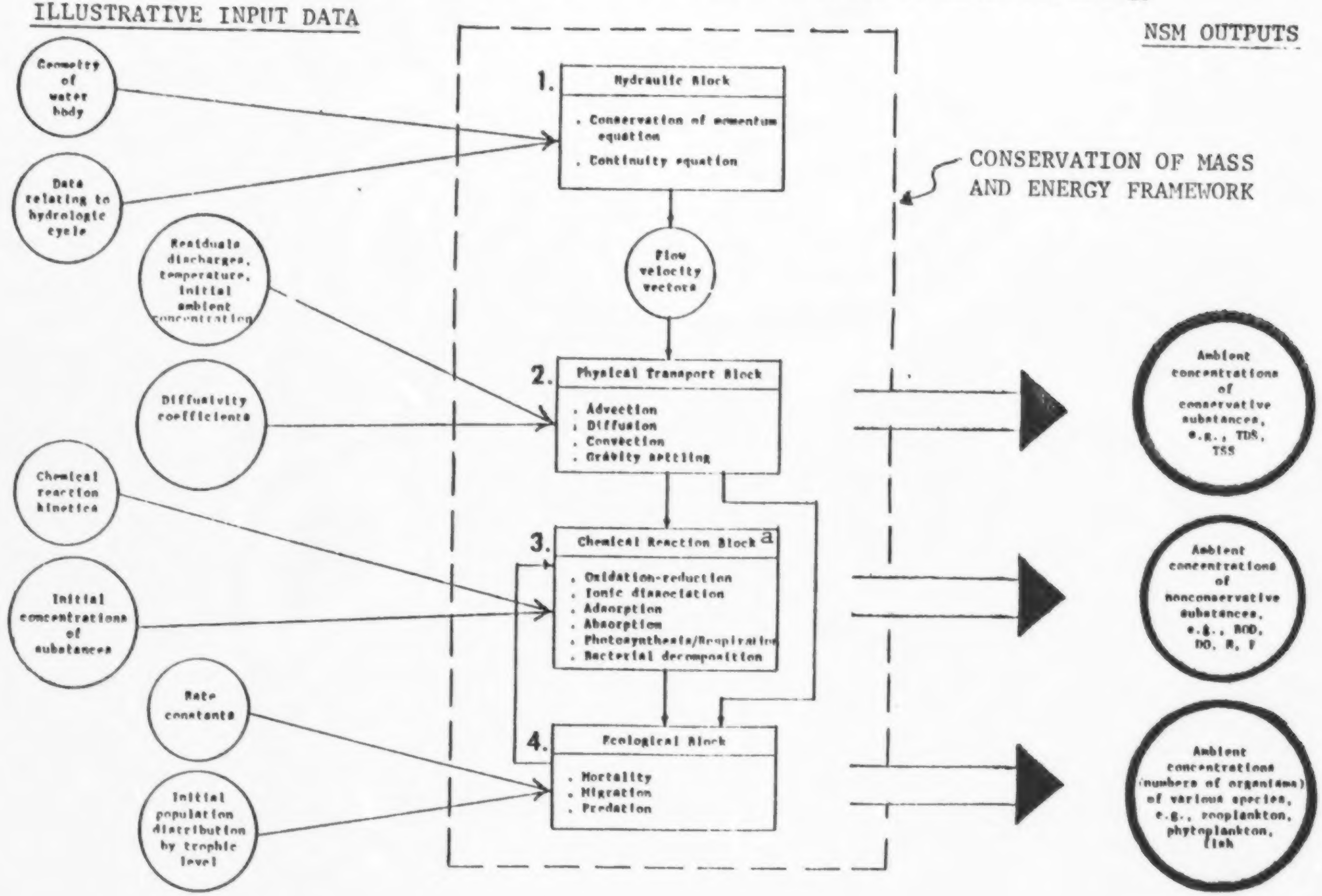
The fourth building block relates to estimating the changes in the biomass or concentration of organisms in different trophic levels in a receiving water body. These changes are the result of: (1) naturally occurring processes over time; (2) residuals which are discharged into a receiving water body and transported (and transformed) throughout the water body; or (3) both (1) and (2). Estimating the changes involves representing mathematically the ecological processes relevant to the species or organisms of interest, given the questions asked. In order to estimate the biomass or concentration of organisms in different trophic levels within the box. equations explaining the ecological processes and interactions must be combined with those of building blocks 1, 2, and 3.

The equations used to represent the processes in each building block and the ways in which these equations are combined and solved depend on the type of water body, flow conditions, problem context, and the assumptions which are made. Figure 4-3 illustrates the relationships between and among the building blocks which comprise receiving water NSMs based on conservation of mass and energy. The following sections briefly describe each of the four building blocks. The descriptions pertain to the case of a one-dimensional river. Introducing additional complexities such as more than one dimension, tidal influences (as in an estuary), and nonsteady-state conditions goes beyond the purposes of this chapter. References containing discussions of additional complexities are cited below.

The Hydraulic Block

The hydraulic block provides the basic information about the rate at which water flows through various parts of a surface water body. For example, if a river were divided into a number of successive segments as shown in figure 4-2, the hydraulic block would provide the velocity and rate of flow with which water moves into and out of each segment. This information can either be: (1) based directly on historical measurements; or (2) computed using a hydraulic model (frequently referred to as a hydrodynamic model). Depending on the context, one method or the other will be preferred. In contexts where no change in factors affecting the flow of water is anticipated, measured historical data can be used as direct input into the other building blocks, providing that the measurements have been taken at locations which coincide with the boundaries of the segments into which the water body is divided for analysis, or that valid correlations can be established for those locations. A model is required when either the physical measures to be applied to residuals generating activities or other factors, e.g., changing levels of activities requiring the diversion of a substantial portion of the flow in the water body, alter the historical

Figure 4-3. Schematic of Receiving Water NSM Based on Conservation of Mass and Energy


ILLUSTRATIVE INPUT DATA
NSM OUTPUTS
CONSERVATION OF MASS AND ENERGY FRAMEWORK
Geometry of water body
Data relating to hydrologic cycle
Residuals discharges, temperature, initial ambient concentration
Diffusivity coefficients
Chemical reaction kinetics
Initial concentrations of substances
Rate constants
Initial population distribution by trophic level
1. Hydraulic Block
. Conservation of momentum equation
. Continuity equation
Flow velocity vectors
2. Physical Transport Block
. Advection
. Diffusion
. Convection
. Gravity settling
3. Chemical Reaction Block a
. Oxidation-reduction
. Ionic dissociation
. Adsorption
. Absorption
. Photosynthesis/Respiration
. Bacterial decomposition
4. Ecological Block
. Mortality
. Migration
. Predation
Ambient concentrations of conservative substances, e.g., TDS, TSS
Ambient concentrations of nonconservative substances, e.g., BOD, DO, N, P
Ambient concentrations (numbers of organisms) of various species, e.g., zooplankton, phytoplankton, fish

[a] Includes chemical, biochemical, and physicochemical reactions.

Abbreviations: TDS, total dissolved solids; TSS, total suspended solids; BOD, biochemical oxygen demand; DO, dissolved oxygen; N, nitrogen; P, phosphorus.

flow characteristics. An example of a physical measure which would alter flow characteristics is dilution. If substantial quantities of water were added to a stream to reduce residuals concentrations, a model would be required to estimate the effect of the additional water on velocities and flow rates. Without such a model, it would be impossible to estimate ambient residuals concentrations using the other building blocks.

Hydraulic models have been extensively developed over the years because of their use in analysis of reservoir construction and operations and in the design of hydraulic structures. In fact, of the four building blocks, the hydraulic block is the one for which model development is most extensive. Most hydraulic models are based on a coupling of the continuity and conservation of momentum equations.[12]

The continuity equation is based on the law of conservation of mass in a fluid element. The equation insures that all water inputs into a receiving water body, and into every segment into which the body may be divided for analysis, equal the outputs. In its simplest form, the continuity equation for a given volume of water may be written as:

$$Q_i - Q_o \pm Q_L + P - E = 0 \quad [4\text{-}1]$$

where:

Q_i = flow into the volume from upstream;

Q_o = flow out of the volume downstream;

Q_L = flow into or out of the volume from lateral sources of withdrawals;

P = precipitation directly onto the volume; and

E = evaporation from the surface of the volume.

Operationally, the continuity equation is usually written as a differential equation. As an illustration of how the continuity equation is derived, the development of the one-dimensional form of the continuity equation for a river is used.

The derivation[13] is based on the river section shown in figure 4-4, for which the following conditions are assumed: nonsteady flow conditions, variable area of river cross-section, constant water density (i.e., no temperature or salinity gradients), and water entering or leaving the river at a uniform rate along the river. Based on equation [4-1], the change in volume of water in the section, ΔV, in a given time interval, Δt, is equal to the sum of all inflows minus the sum of all outflows. Expressed mathematically and using the notation shown in figure 4-4 yields:

[4-2]

$$\Delta V = \overset{\text{Inflow}}{\overset{\downarrow}{Q\Delta t}} + \overset{\text{Lateral flow}}{\overset{\downarrow}{q\Delta x\Delta t}} - \overset{\text{Outflow}}{\overset{\downarrow}{\left(Q + \frac{\partial Q}{\partial x}\Delta x\right)\Delta t}}$$

$$= q\Delta x\Delta t - \frac{\partial Q}{\partial x}\Delta x\Delta t$$

where: ΔV = change in volume = $\Delta A\Delta x$;

A = cross-sectional area;

Δx = length of section;

Q = rate of inflow from upstream section;

q = rate of inflow per unit distance along the section; and

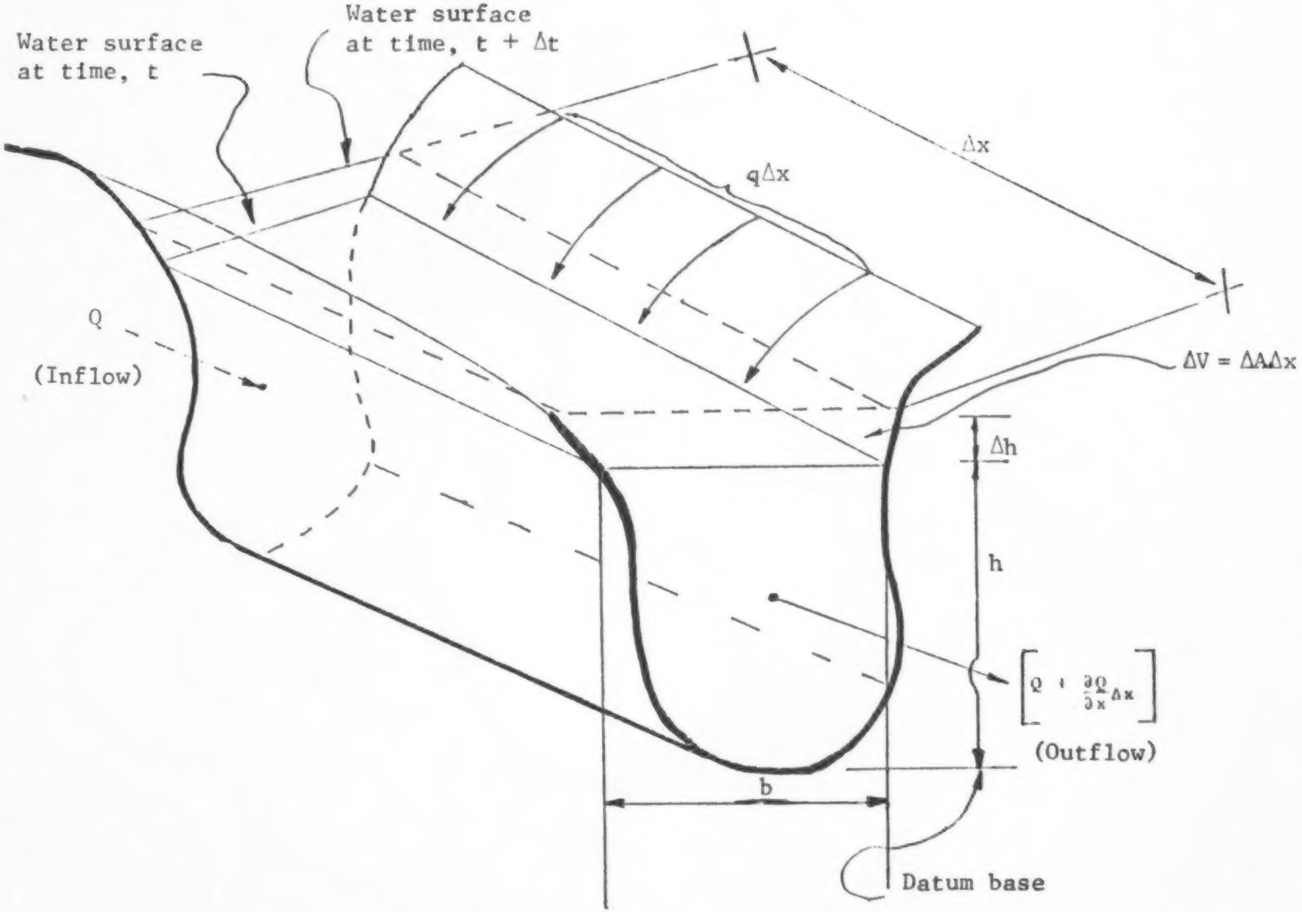
$\left(Q + \frac{\partial Q}{\partial x}\Delta x\right)$ = rate of outflow to downstream section.

Substituting $\Delta A\Delta x$ for ΔV on the left side of equation [4-2], dividing both sides of the equation by $\Delta x\Delta t$, and taking the limit as $\Delta t \to 0$, yields:

$$\frac{\Delta A}{\Delta t} = \frac{\partial A}{\partial t} = q - \frac{\partial Q}{\partial x} \qquad \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} - q = 0$$

$$\lim \Delta t \to 0$$

Figure 4-4. Diagram of River Section for Development of Continuity Equation


Water surface at time, t
Water surface at time, t + Δt
Δx
qΔx
ΔV = ΔAΔx
Q
(Inflow)
Δh
h
$\left[Q + \frac{\partial Q}{\partial x}\Delta x\right]$
(Outflow)
b
Datum base

Rearranging terms and making the following approximation (see figure 4-4):[14]

$$\frac{\partial A}{\partial t} = b\frac{\partial h}{\partial t}$$

where b is the width of the river at the water surface, the instantaneous one-dimensional form of the continuity equation for a river or stream may be expressed as:

$$[4\text{-}3] \qquad b\frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} - q = 0$$

Given that a continuity equation can be formulated for a river or stream, the principle of conservation of momentum is used to derive the equation of motion. The equation of motion determines the velocity with which water moves through segments of the water body. Momentum, M, is defined as the product of mass, m, and its velocity, U, that is M = mU. The prinicple of conservation of momentum states that the time rate of change of momentum of a moving fluid particle is equal to the sum of the forces acting on the particle (Newton's Second Law of Motion). The differential equation which expresses this principle is termed the equation of motion.

Newton's Second Law of Motion for the time rate of change of momentum in the x-direction can be expressed mathematically as:

$$[4\text{-}4] \qquad \frac{dM}{dt}\, x = \Sigma F_x$$

where $\frac{dM}{dt}\, x$ is the instantaneous change in momentum in the x-direction and F_x is the sum of the external forces acting in the x-direction. Combining equation [4-4] with the definition of momentum (M = mU) yields the general momentum form of Newton's Second Law:

$$[4\text{-}5] \qquad \frac{d(mU)}{dt}\, x = m\frac{dU}{dt}\, x + U_x\, \frac{dm}{dt} = \Sigma F_x$$

This equation is the basis for the equations of motion developed for receiving water bodies. In order to develop a motion equation from equation [4-5] the left-hand side of the equation, $\frac{d(mU)}{dt}x$, must be modified to account for the sum of momentum and its components, and expressions derived for the external forces (ΣF_x) acting on the fluid elements. Equation [4-6] below is the instantaneous equation of motion, derived from equation [4-5], for nonsteady state flow in the x-direction for a one-dimensional river.

[4-6]
$$\frac{\partial Q}{\partial t} + Q\frac{\partial U}{\partial x} + U\frac{\partial Q}{\partial x} + gA\frac{\partial h}{\partial x} + gA\,\frac{U}{KR^{\alpha}}^{\,2} = 0$$

where: Q = rate of inflow from stream section;
U = velocity in the x-direction;
g = acceleration due to gravity;
A = cross-sectional data;
h = depth
K and α = empirical constants; and
R = hydraulic radius, i.e., A divided by the wetted perimeter.

Simultaneous solution of equation [4-3], the continuity equation, and equation [4-6], the momentum equation, will produce the velocity information required as inputs into the other receiving water model building blocks for analyzing a one-dimensional river. The equations are typically solved using finite difference numerical integration methods. A river being analyzed would be divided into segments similar to the segments shown in figure 4-2 and, given the geometry of each segment, the equations solved simultaneously for all segments.

Additional information on the hydraulic block and the formulation of hydrodynamic models is contained in, for example, chapter 2 of Tracor, Inc., (1971).

The Physical Transport Block

The physical transport block of a receiving water model analyzes the movement of materials within the water passing through a receiving water body. This analysis requires information from the hydraulic block with respect to the quantity and velocity of water movements at a number of locations, the number depending on how the water body is segmented for analysis. Given this information, and values for the diffusion coefficients,[15] the physical transport block estimates ambient concentrations of conservative residuals discharged into a water body. It also provides the transport information for estimating ambient concentrations of nonconservative residuals and the impacts of both conservative and nonconservative residuals on living organisms, by blocks 3 and 4, respectively.

As indicated in the previous section, a number of physical processes affect the movement of materials in water, the two most important being advection and diffusion, where diffusion is really a combination of several different diffusion-type processes. These processes are discussed earlier in this chapter and in chapter 2. The mathematical formulation of the conservation of mass or energy equation relating to these processes is contained in pages 50 through 54 of chapter 2. However, some additional comments[16] are warranted here. For any given control volume, the advection-diffusion equation can be stated:

$$
\begin{aligned}
\begin{matrix}\text{Average rate of}\\ \text{change of mass}\end{matrix} &= \begin{matrix}\text{Average rate of inflow}\\ \text{due to advection}\end{matrix} - \begin{matrix}\text{Average rate of outflow}\\ \text{due to advection}\end{matrix}\\
\text{[4-7]} \qquad &+ \begin{matrix}\text{Average rate of inflow}\\ \text{due to diffusion}\end{matrix} - \begin{matrix}\text{Average rate of outflow}\\ \text{due to diffusion}\end{matrix}\\
&+ \text{Exogenous inputs}
\end{aligned}
$$

For the one-dimensional river, the differential form of equation [4-7] can be reduced to:

[4-8]
$$\frac{\partial c}{\partial t} = -U\frac{\partial c}{\partial x} + k_x\frac{\partial^2 c}{\partial x^2} + E$$

where: c = cross-sectional average concentration of the residual of interest;

t = time;

x = longitudinal distance along river;

U = average velocity = Q/A;

Q = flow rate;

A = cross-sectional area;

k_x = effective or apparent diffusion coefficient in the x direction; and

E = sum of all sources, sinks, boundary inflows/outflows, and interactions among residuals.

The source-sink term, E, includes processes such as deposition, distributed (e.g., lateral) inflows, and first-order decay, reaeration, and residuals interactions. These are processes which affect nonconservative residuals and relate to the chemical reaction block. For additional discussion, particularly regarding the two-and three-dimensional cases, see Thomann (1972) and Tracor, Inc. (1971).

For a given river or stream for which requisite hydraulic information is available, equation [4-8] can be applied in one of two ways, depending on the context. The first is where the river or stream to be studied is divided into a finite number of discrete segments. This approach is implicit in most of the material presented in this chapter, and most currently operational receiving water models are formulated on this basis.

The extent of segmentation required for any given application (questions being asked) depends on: the number of residuals dischargers, water inflows/outflows along the river or stream, or both; the related flow conditions; and the required spatial pattern of estimates of ambient concentration.

The second is where no segmentation is applied. This approach is typically employed to estimate the downstream impacts of residuals discharged from a single source, or a number of sources discharging at one location. The assumptions required to apply equation [4-8] in this manner are more constraining than if the finite segment approach were used, primarily because the segmented approach enables variable sets of conditions to be explicitly included, one set for each segment.[17]

Equation [4-8] is a parabolic, linear, partial differential equation and can be solved either analytically or numerically, as indicated in chapter 2. Many analytical solutions are available in the literature, such as in Carslaw and Jaeger (1959), Cranik (1956), and Tracor, Inc. (1971).

One frequently employed analytical solution to equation [4-8] is known as the Gaussian. This solution is given in many texts, e.g., Carslaw and Jaeger (1959), Daily and Harleman (1966). For conservative residuals, e.g., suspended solids, the solution is:

$$[4\text{-}9] \qquad C = \frac{Me^{-\frac{(x-Ut)^2}{4k_x t}}}{A \quad 4k_x t}$$

where C = concentration, mass per unit volume, M = mass, and the other variables are defined as for equation [4-8]. This solution assumes that a quantity of conservative material, a "slug," is instantaneously released into a river. Equation [4-9] is referred to as a Gaussian solution because when concentration, C, is plotted as a function of distance downstream, x, with t held fixed, the resulting distribution is a Gaussian distribution as shown in figure 4-5B for the river reach shown in figure 4-5A. The advective transport of the slug (movement downstream) and the diffusion (spreading) as the slug progresses downstream are apparent from the figure.

In actual rivers and streams, the Gaussian solution to the one-dimension advection/diffusion equation is valid only to a distance downstream from the point of injection to the point where no significant variations in concentration exist across the cross section. That means to the point where there is no longer any diffusion of the injected material. This has been termed the "diffusive period" by Fischer (1967, 1973).

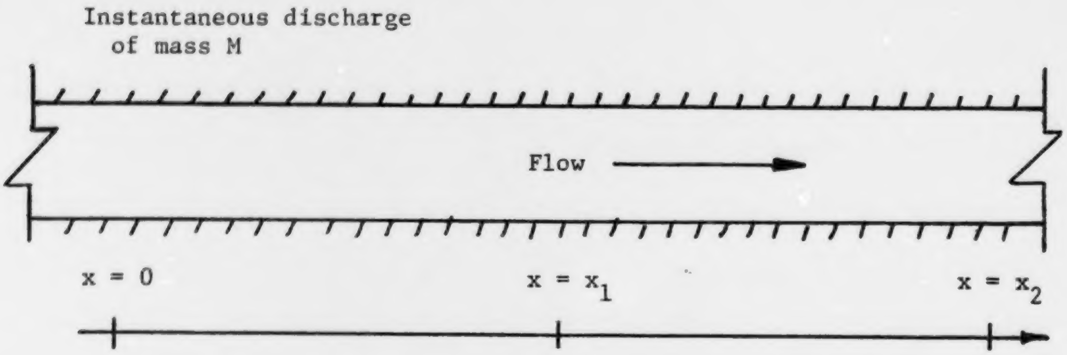
Receiving water models which are composed only of blocks 1 and 2 deal primarily with analyzing salinity (total dissolved solids) and sediment (total suspended solids) transport problems described earlier. However, most currently operational receiving water models are composed of blocks 1, 2, and 3, the last being the chemical reaction block.

The Chemical Reaction Block

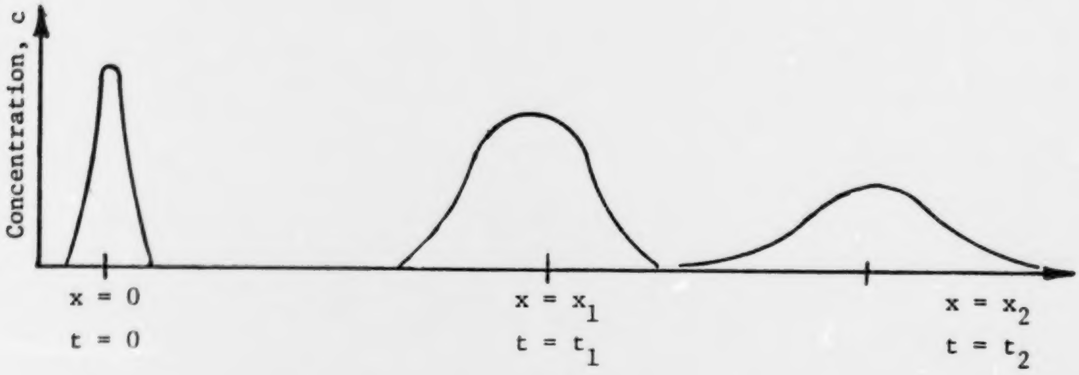
To this point, receiving water models have been discussed only in terms of the flow of water and materials within a water body. Thus, they include only materials that do not react with other substances, do not undergo transformations, and are not exchanged across designated boundaries of control volumes by processes other than advection and diffusion. In the real world, however, there are substantial transformations of some forms of mass through chemical and biological processes, as well as significant exchanges of gases across liquid-gas interfaces (physicochemical processes), e.g.,

Figure 4-5. Illustration of Gaussian Distribution

A. Schematic of Hypothetical River


Instantaneous discharge
of mass M
Flow
x = 0
x = x1
x = x2

B. Distribution of Concentrations at Indicated Cross Sections in Relation to Distance from Discharge Point



sedimentation and scour. The chemical reaction block, in combination with the hydraulic and physical transport blocks, attempts to model these processes quantitatively.

However, this is a difficult and complicated task because of the vast array of organisms and chemical elements and compounds dispersed throughout a water body, and the reactions among them. Many of the elements and compounds, and many of the organisms, undergo a number of reactions. Some of these reactions occur in multiple steps producing a large number of intermediate products and reactants. (For examples see table 4-1 on page .) To account for the temporal and spatial distribution of each of these elements, compounds and organisms by constructing a mass balance for each, with the inclusion of rate terms for each possible reaction as a source or sink, is beyond existing computational ability. It is also limited by the existing knowledge of each substance, its possible reactions, and the expense of measuring its concentrations in the environment.

Consequently, a number of practical expedients have been taken to make the chemical reaction and ecological blocks of receiving water models tractable, including: (1) grouping classes of compounds and organisms such as carbohydrates, nitrogenous organics, zooplankton, and phytoplankton; (2) considering only the most important materials, organisms, and reactions; (3) including only overall reaction processes (simplified kinetics), using empirically derived expressions for estimating their rates, as illustrated in Zison, et al. (1978); and (4) using operational surrogates to reflect concentrations of aggregated classes of materials, e.g., biochemical oxygen demand for biodegradable organics.

In the previous section, it was indicated that the chemical, biochemical, and physicochemical processes which affect the transformation of residuals as they are transported could be incorporated into the "E" term, e.g., the sum of sources, sinks, and residual interactions, of the advection/diffusion physical transport equation (equation [4-8]). To illustrate how this is accomplished, a steady-state dissolved oxygen (DO) model of the Streeter-Phelps variety is used. This model employs two linear differential equations, one for biochemical oxygen demand (BOD) and one for dissolved oxygen (DO). Streeter-Phelps equations of one form or another are found in Phelps (1953), Dobbins (1964), Hydroscience (1971). In this model, BOD and DO are the endogenous variables; all other sources and sinks are exogenous variables. The desired outputs of this type of model are DO concentrations throughout a river or stream.

DO in a water body is used in oxidizing organic material, in this case measured as BOD, much of which is discharged into water bodies as residuals from man's activities. Oxygen is replenished by reaeration through the air-water interface and by photosynthesis. The basic differential equations which describe the time rate of change of BOD and DO in a unit volume, due only to chemical and biological activity are, respectively:[18]

$$\frac{dL}{dt} = -K_1L + \Sigma S\text{, and} \tag{4-10}$$

$$\frac{dD}{dt} = -K_1L + K_2(D_s - D) + \Sigma S \tag{4-11}$$

where: L = biochemical oxygen demand, mg/l;

D = dissolved oxygen level, mg/l;

D_s = dissolved oxygen saturation level, mg/l;

K_1 = BOD rate constant, per day;

K_2 = reaeration rate constant, per day;

S = other sources and sinks of organic material and oxygen, mg/l; and t = time.

The ΣS term represents the sources and sinks of organic material and dissolved oxygen which are treated as exogenous inputs. Resuspension and sedimentation are examples of sources and sinks of organic material, respectively. Photosyntetic activity and benthal demands are examples of sources and sinks of dissolved oxygen, respectively.

Combining equations [4-10] and [4-11] with equation [4-8] and assuming steady-state conditions yields an equation set which takes into account both the physical transport of DO and BOD (blocks 1 and 2) and the chemical and biological interactions which take place between them as they are transported (block 3). This set is:

[4-12] $$0 = k_x \frac{d^2L}{dx^2} - U\frac{dL}{dx} - K_1L + \Sigma S, \text{ and}$$

[4-13] $$0 = k_x \frac{d^2D}{dx^2} - U\frac{dD}{dx} - K_1L + K_2(D_s-D) + \Sigma S$$

where the variables are as defined earlier. The unknowns in equations [4-12] and [4-13] are L and D, representing BOD and DO, respectively. The mean downstream velocity, U, and the longitudinal dispersion coefficient, k_x, are exogenously determined. The mean velocity, U, is determined either by measurement or from a hydraulic model, depending on a number of factors as indicated in the discussion of the hydraulic block. These equations can be solved by either analytical or numerical integration, just as can the equations for the hydraulic and physical transport blocks. The original formulation by Streeter and Phelps was solved by analytical integration.

The above illustrates the principal way in which the chemical reaction, physical transport, and hydraulic blocks are combined in a receiving water model. Depending on the number of reactions to be considered, physical transport and chemical reaction rate equations would be combined into equation sets as shown above. The BOD-DO case is an example of a two-stage reaction, hence two equations are required. If a four-stage reaction, e.g., nitrification (organic nitrogen → ammonia nitrogen → nitrite → nitrate nitrogen), were to be combined with the physical transport equation, then a set of four differential equations would be required.

The Ecological Block

The ecological block of a receiving water model, in conjunction with the hydraulic, physical transport, and chemical reaction blocks, is used to estimate the spatial and temporal distributions of relevant organisms residing in a water body, and the effects various levels of residuals discharges have on those distributions. An ecological block is composed of a set of differential equations which attempt to account quantitatively for the biological/ecological functions which affect the location and population levels of specified organisms. Relevant functions include growth, respiration, death, predation, excretion, and feeding. Receiving water models which contain an ecological block are considerably more complex than those that do not. Depending on the number of ecological linkages considered, they are often referred to as aquatic ecosystem models.[19]

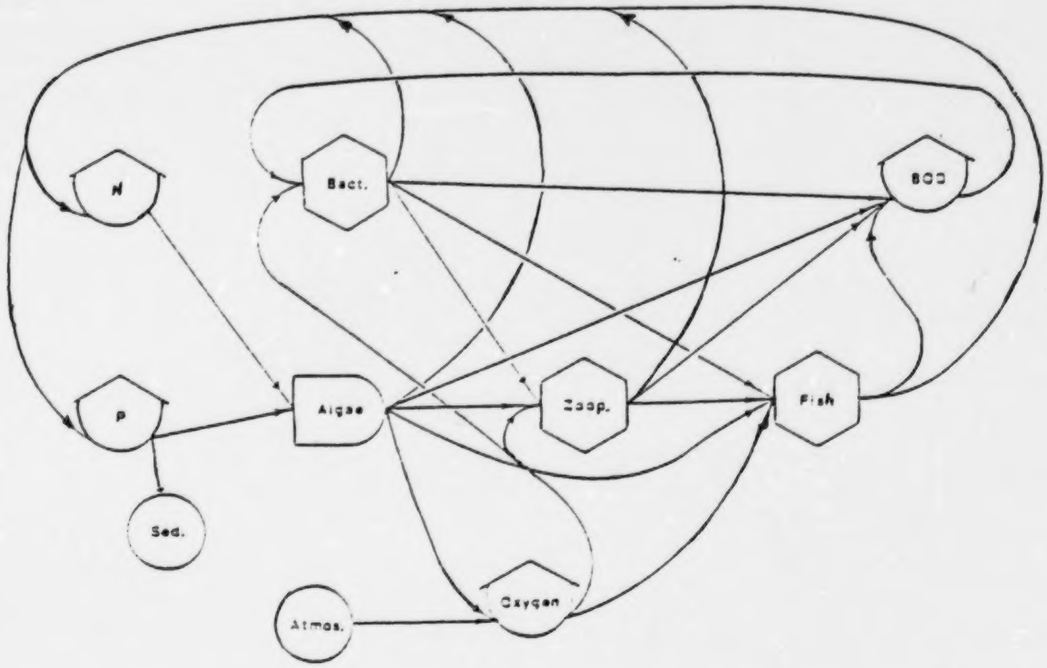
The principle of conservation of mass is used to formulate the equations in the ecological block, in much the same way the principle is used in the chemical reaction block. The equations are expressed in terms of rates of change of the relevant functions in relation to a control volume.

The relationship between the chemical reaction and ecological blocks is important. In a receiving water model which contains a complex ecological block, the demarcation between the chemical reaction and ecological blocks may not be readily discernible. This is because the uptake and production of chemical compounds by organisms must be considered in the mass balances regarding a given compound, at the same time the availability of a given compound must be considered in the growth computation of the mass balance calculation for a given organism. In other words, there are numerous linkages among the physical, chemical, and biological/ecological processes at work in a water body. Figure 4-6 illustrates this point by showing the material flows between relevant compounds and organisms defined for each control volume, or reach, in an aquatic ecosystem model of the Delaware Estuary (Kelly, 1975).

As implied above, ecological blocks of receiving water models vary in complexity. In some cases they contain only a few rate equations for aggregate classes of organisms, with few or no explicit feedback mechanisms among organisms or between chemical compounds. In other cases, such as shown in figure 4-6, numerous pathways and rates are explicitly specified among organisms and between organisms and chemical compounds.

In models in which a number of chemical compounds and organisms are considered explicitly, each compound and each organism, or each class of compounds and each class of organisms, is referred to as a "compartment." For example, the aquatic ecosystem shown in figure 4-6 is composed of eight compartments. (The circles Sed. [sediment] and Atmos. [atmosphere] are not considered compartments. They represent, respectively, a sink and a source.) Applying the mass balance principle to the ecological block requires that a mass balance equation be written for each compartment specified in an aquatic ecosystem for each segment into which the water body is divided for analysis. Therefore, in order to quantify mathematically the ecosystem shown in figure 4-6, a mass balance equation must be written for

Figure 4-6. Material Flows Within one Reach of Aquatic Ecosystem Model for the Delaware Estuary



Abbreviations: N, nitrogen; P, phosphorus; Bact., bacteria; BOD, biochemical oxygen demand; Sed., sediment; Atmos., atmosphere; Zoop., zooplankton.

Source: Robert A. Kelly, "The Delaware Estuary," in Clifford S. Russell, ed., Ecological Modeling in a Resource Management Framework, RFF Working Paper QE-1 (Washington, D.C., Resources for the Future, 1975) p. 111.

each of the compartments shown. Figure 4-7 summarizes the differential equations developed by Kelly (1975) for each compartment of the ecosystem shown in figure 4-6 plus equations for three endogenous variables--suspended solids, toxics, and temperature--which are assumed to affect the rates of material transfers among the compartments.

Each of the variables on the right-hand sides of the equations shown is itself represented by an equation. For example, the mass balance equation for algae is composed of six separate equations, one each for feeding, respiration, death, excretion, predation, and physical transport. These equations are referred to as rate equations. The transport equations for each compartment and each endogenous variable, denoted by subscript T, actually represent the hydraulic and physical transport blocks and are identical with the advection/diffusion equation presented earlier. The endogenous variables are inputs to the rate equations included in the equations for individual compartments.

Aquatic ecosystem models of this type must be solved by dividing the water body to be analyzed into segments (control volumes) and using numerical integration methods. Solution of aquatic ecosystem models is further complicated by the fact that the differential equations posited for the compartments are typically nonlinear.

In general, the ecological block of most receiving water models is still rather crude in relation to the other building blocks. Nevertheless, many current aquatic ecosystem models--such as the model described above--appear to have a rigorous and comprehensive mathematical structure. However, the ecological components of these models are more often than not impossible to verify. Verification is a problem because of the many assumptions that must be made regarding the variables affecting a given compound

Figure 4-7. Equation Set for Eight Compartment Aquatic Ecosystem Model

Differential equations for each compartment, for each unit volume:

(1) Algae, A, mg/l $\frac{dA}{dt} = f_A - r_A - d_A - e_A - p_A + T_A$

(2) Zooplankton, Z, mg/l $\frac{dZ}{dt} = f_Z - r_Z - d_Z - e_Z - p_Z + T_Z$

(3) Bacteria, B, mg/l $\frac{dB}{dt} = f_B - r_B - d_B - e_B - p_B + T_B$

(4) Fish, F, mg/l $\frac{dF}{dt} = f_F - r_F - d_F - e_F$

(5) Oxygen, $\underline{O}$, mg/l $\frac{dO}{dt} = 2.319(f_A - r_A - r_A - r_A - r_A) + \alpha T_{\underline{O}} + i_{\underline{O}}$

(6) BOD, L, mg/l $\frac{dL}{dt} = d_A + e_A + d_Z + e_Z + d_B + e_B + d_F + e_F - f_B + T_L + i_L$

(7) Nitrogen, N, mg/l $\frac{dN}{dt} = 0.1087(r_A + r_Z + r_B + r_F - f_A) - \beta + T_N + i_N$

(8) Phosphorus, P, mg/l $\frac{dP}{dt} = 0.02174(r_A + r_Z + r_B + r_F - f_A) - \gamma + T_P + i_P$

Differential equations for endogenous variables:

(1) Suspended Solids, σ, mg/l $\frac{d\sigma}{dt} = -\delta + T_\sigma + i_\sigma$

(2) Toxics, ϕ, mg/l $\frac{d\phi}{dt} = -\varepsilon + T_\phi + i_\phi$

(3) Temperature, ∂, °C $\frac{d\partial}{dt} = -\zeta + T_\partial + i_\partial$

where:
f = feeding,
p = predation,
r = respiration,
d = death,
e = excretion,
T = transport,
α = reaeration,
β = nitrification,
γ = precipitation,
δ = sedimentation,
ε = toxics decay, and
ζ = heat exchange.
i = input from industrial, municipal, or tributary sources,

Inputs of residuals: lbs/day: BOD, N, P, Toxics, Suspended Solids
Btu: Heat

Source: Robert A. Kelly, "The Delaware Estuary," in Clifford S. Russell, ed., Ecological Modeling in a Resource Management Framework (Washington, .C., Resources for the Future, 1975) modified from figure 4, p. 116.

or organism and the rate equations relating thereto, and the inability to collect the vast amount of data necessary for verification. Consequently, although most of the receiving water models summarized in Appendix A contain the potential ability to generate information on some biological/ecological effects, this capacity should be viewed at this time with a certain degree of skepticism. For additional information on the ecological block of receiving water models see Scavia and Robertson (1979), Wiley (1975), Middlebrooks, et al. (1974), and Russell (1975).

Statistical Approach for Analyzing Receiving Water Bodies

The statistical approach for analyzing receiving water bodies is essentially the same as the general statistical approach for analyzing natural systems described in chapter 2. Hence, the purpose of this section is to illustrate briefly some applications of the statistical approach in the analysis of receiving water bodies.

Statistical methods have had and continue to have considerable use in the analysis of receiving water bodies. However, as more has become known about water quality problems and the natural processes which affect them, the use of receiving water NSMs based on the statistical approach has declined markedly. This is because receiving water NSMs based on the statistical approach do not explain causal relationships and because the range over which they can make predictions is basically limited to the range represented by the sample on which any given statistical NSM is based. Nevertheless, because of their simplicity, receiving water NSMs based on the statistical approach continue to have utility in certain REQM contexts. Examples are: (1) where a first cut, crude analysis is required; and (2) where the detailed quantitative data necessary to apply a more complex model based on conservation of mass and energy are not available, but some analysis is essential.

The principal statistical method employed in receiving water NSMs is regression analysis, although other methods have also been applied.[20] In regression analysis, a dependent variable, Y, is expressed as a function of some number of independent variables, X_i, each times a coefficient, B_i, plus a random disturbance term, E, assuming some structural form, e.g., linear, semi-log, log-log. The most common form of the regression equation is multiple linear, the term "multiple" indicating that more than one independent variable is included in the equation. This equation is of the form, $Y = a + B_1X_1 + . . . + B_nX_n + E$, where a is a constant (the intercept).

Receiving water NSMs based on regression analysis have been applied primarily to two types of receiving water bodies, estuaries and lakes or impoundments.[21] Significantly more applications have been made to lakes and impoundments than to estuaries. Four brief descriptions follow which illustrate ways in which regression analysis has been used in analyzing water quality in these two types of receiving waters.

One observation about the examples should be noted. The two examples relating to estuaries are both regression analyses based on time series data; the two examples relating to lakes are both regression analyses based on cross-sectional data. Regression analyses of estuaries are usually based on time series data because every estuarine system is essentially unique, regardless of geographical location. Therefore, regression analyses of estuaries based on cross-sectional data would not be likely to produce relationships which would be both statistically significant and have some rational explanation based on knowledge of the phenomena analyzed.

Regression analyses of lakes can be based on either time series data or cross-sectional data. Lakes in similar geographic settings and climatic zones display many common ambient water quality conditions. Regression analyses of lakes using cross-sectional data are quite common because it is often easier to obtain several observations about many similar lakes than many observations, over time, of a single lake.

Examples of Regression Analyses of Water Quality in Estuaries

The two analyses of water quality in estuaries attempted to develop relationships to predict the concentration of coliform organisms. Coliform organisms are an indicator of discharges of fecal material into water bodies. Both analyses used regression methods, but each examined the problem in a different way. In the first, the researchers began by assuming that they knew very little about the factors influencing coliform concentration in the estuary. Regression analysis methods were used to help identify the important factors. Then, given those factors, a relationship (equation) to predict coliform concentration was developed. The second example assumed the form of the relationship between coliform concentration and some independent variables and used regression methods only to estimate a set of coefficients for the relationship.

The first example is an analysis by Kelch and Lee (1978) of the Tillamook estuary in Oregon. Kelch and Lee first identified 135 independent variables which might have an effect on fecal coliform concentrations in the estuary. These variables were basically variations on a limited number of variables such as: the quantities of water entering the estuary from tributaries; fecal coliform concentrations in the tributaries; precipitation; tide levels; water temperature; concentrations of bacteria other than fecal coliform; and time. Additional variables were formulated specifying different aggregations of the data relating to each of these variables and specifying relationships with the created variables in both log and non-log forms. For example, variables formulated based on temperature data included: low temperature on the sample day; high and low temperatures on the day previous to the sample day, and the logs of each; average minimum, average maximum, and average temperature of the previous month, and the logs of each.

The approach Kelch and Lee used was to do two separate sets of regression analyses. In each set two groups of regressions were performed, one using observed values over time of the dependent variable, fecal coliform count (Y), and of the independent variables, the other using the logs of these values.

The fecal coliform count of the estuary is defined as the mean of the data for four sampling points in the estuary. The first set of regressions consisted of simple regressions between Y and Log Y and each of the posited independent variables (720 regressions). These simple regressions were of the following forms: $Y = a + BX + E$; $Y = a + B \log X + E$; $\log Y = a + BX + E$; and $\log Y = a + B \log X + E$.

The purpose of this set of regressions was to identify which variables were strongly associated with fecal coliform concentration and therefore should be studied further in the next set of regressions. Based on a standard statistical test--the F-test at 90% confidence level--Kelch and Lee eliminated all but 26 of the original 135 variables.

The second set of regressions consisted of regressing Y against the 26 remaining independent variabels, and then Log Y against the same set of variables. The form of the equations is similar to the multiple linear case shown above, the only difference being that the independent variables are in both log and non-log forms. Both groups of regressions were run using a stepwise procedure.[22] The final result of a stepwise procedure is the regression equation comprised of the independent variables which best predict the dependent variable, given a prespecified acceptable level of significance.

Using the stepwise procedure, Kelch and Lee found the two best regression equations, one which best predicts fecal coliform concentration in the estuary, the other which best predicts the log of fecal coliform concentration in the estuary, given the variables investigated and the level of significance specified. These equations are:

$$Y = -2.63 + 0.44X_2 + 3.27X_{94} - 0.022X_{96} \tag{4-14}$$

$$\text{Log } Y = 16.6 - 0.036X_2 - 8.88X_{28} + 0.057X_{48} \tag{4-15}$$

where: Y = fecal coliforms/100 ml;

X_2 = fecal coliforms /100 ml in the Trask River (a tributary of the estuary);

X_{28} = the log of highest temperature (°F) on the previous day;

X_{48} = the percent resistance to fecal coliform to procaine penicillin G in the Kilchis River (a tributary of the estuary);

X_{94} = the percent resistance of fecal coliform to Kanamycin biota from all sources; and

X_{96} = the amount of salmon in the Kilchis River.[23]

A few comments are warranted regarding the utility of the equations derived for predicting fecal coliform concentration in the Tillamook estuary. First, neither of these equations can be used to predict the spatial distribution of fecal coliform concentrations in the estuary. Second, because the time series data used covered only a short period--October 19, 1975 through March 19, 1976--it is uncertain whether the relationships developed would be valid under conditions which were not essentially the same as those during this period. Third, the variables which are included in the equations make it very difficult, perhaps impossible, to analyze the effects of REQM strategies on fecal coliform concentration in the estuary. This is because only a few variables which could be affected--directly or indirectly--by REQM strategies were included in the original specification of independent variables. The primary usefulness of the statistical NSM derived may be the clues it provides about factors affecting fecal coliform concentration in the receiving water body which should be included in a conservation of mass and energy NSM of the estuary. It should be pointed out that Kelch and Lee were well aware of the shortcomings of the equations produced, and viewed their work only as a preliminary screening analysis.

The second illustration is a statistical NSM posited by Diachishin (1957) for predicting coliform concentration in New York Harbor. Diachishin assumed that coliform concentration in the estuary varied with the tidal cycle and posited the following relationship:

$$Y = K_1 + K_2 \sin \frac{t - t_0}{p} \qquad [4\text{-}16]$$

where: Y = the log of fecal coliforms/100 ml;

K_1, K_2, and t_0 = constants;

p = the duration of the tidal cycle (12.38 hrs.); and

t = time, hours after beginning of tidal cycle.

Expanding the expression sin $\frac{t - t_0}{p}$ in equation [4-16], Diachishin arrived at the following equation to predict coliform concentration at a given location in the estuary:

$$[4\text{-}17] \qquad Y = K_1 + K_3 \sin \frac{t}{p} + K_4 \cos \frac{t}{p} \ .$$

K_1, K_2, and K_4 were then interpreted to be regression coefficients to be estimated. Given a sufficient number of observations of Y, concentration of coliform, and times after the beginning of the tidal cycle, t, the regression coefficients can be estimated. As indicated, the model was applied to New York Harbor. Equation [4-17] has served as the basis for several other similar statistical NSMs for tidal estuaries (Pyatt, 1964).

Because equation [4-17] is a regression equation, it has the same general limitations as Kelch and Lee's equations, equations [4-14] and [4-15]. More important, there are no variables in the equation which can reflect REQM strategies. Steady-state conditions are implied, and the equation provides no means of estimating the effects of reducing the discharge of fecal coliforms into New York Harbor.

Examples of Regression Analyses of Water Quality in Lakes

The majority of statistical NSMs of lakes based on regression analysis have focused on eutrophication. The two examples described below deal with eutrophication, utilizing cross-sectional data, but analyze the eutrophication problem in slightly different ways.

The first example is a set of regression equations developed by Shannon and Brezonik (1972a) to predict the level of eutrophication in lakes in relation to nitrogen and phosphorus loading rates, grams per cubic meter of lake volume per year. The regression analysis was based on data on nitrogen and phosphorus loadings and on a number of other factors relating to the level of eutrophication for 55 lakes located in north central Florida. Level of eutrophication is measured by a "trophic state index" (TSI) which is comprised of a combination of seven variables: primary production, chlorophyll a; total phosphorus; total organic nitrogen; secchi disc measurement; specific conductivity; and Pearsall's cation ratio.[24]

Shannon and Brezonik posited several different relationships relating phosphorus and nitrogen loadings to the tropic state index (TSI).[25] Each relationship was in the form of a multiple regression with TSI as the dependent variable and either an additive or multiplicative combination of nigrogen, N, and phosphorus, P, loadings as the independent variables. Each regression analysis was run using a stepwise regression procedure, as described in the previous section, based on data developed for each of the 55 lakes. The analysis produced the following equations:

[4-18] $TSI = 26.11(P) + 0.90(N)$ [R = 0.79]

[4-19] $TSI = 48.86(P) - 5.26(N)(P) + 0.83(N)$ [R = 0.81]

[4-20] $TSI = 26.10 + 242.36(P)^2 + 1.12(N)^2 + 28.86(N)(P) + 2.37(N)$ [R = 0.83]

[4-21] $TSI = 0.19 \frac{N}{P}$ [R = 0.63]

[4-22] $TSI = 1.08(P)^{0.92} \cdot (N)^{0.04}$ [R = 0.62]

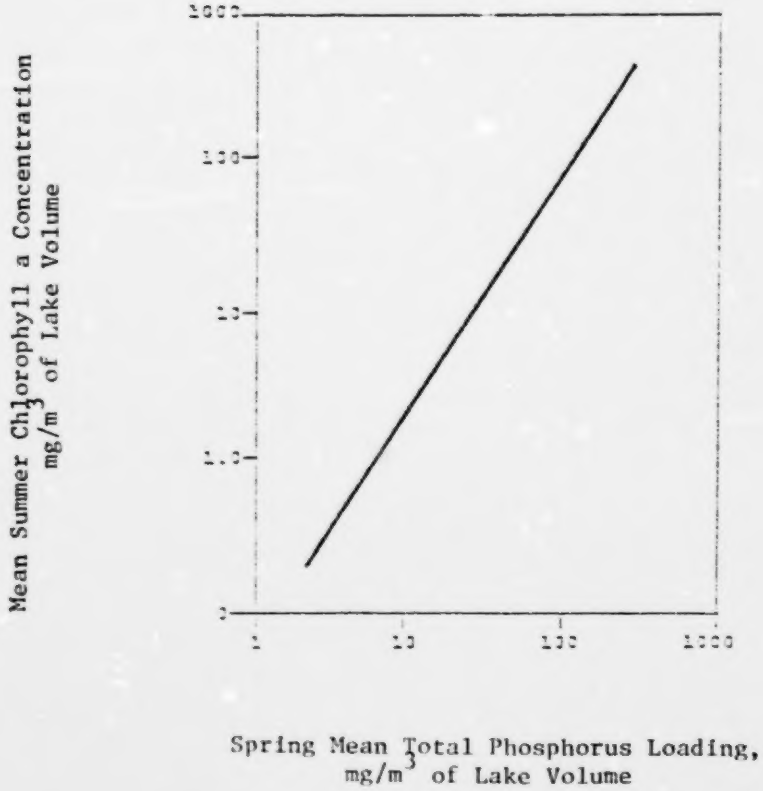
N and P are in grams per cubic meter of lake volume per year. The bracketed R to the right of each equation is the multiple correlation coefficient, significant at the 99% confidence level. A comparison of TSI values estimated using equation [4-20] with empirically determined values indicated that the average error of estimated values was about ± 25 percent.

Shannon and Brezonik noted that equation [4-18], which incorporates no interactives forms of the N and P loading variables, is almost as significant as equations [4-19] and [4-20], which include interactive N and P terms. Hence, inclusion of the interactive terms only marginally improves predictive power. They also deduced that because equations [4-21] and [4-22], containing multiplicative relationships, are the least significant of the equations the effect on eutrophication of nitrogen and phosphorus loadings may be additive, but with one nutrient having more influence than the other. Further, the fact that the P loading variable is always brought into the equations first by the stepwise regression procedure suggests that phosphorus is likely to be the limiting nutrient in the eutrophication process in the 55 lakes sampled. These results have direct implications for developing REQM strategies, which, for example, could be directed toward reducing P loadings.

The second example is a regression analysis done by Dillon (1974). He developed a relationship which is potentially more useful for analyzing eutrophication in lakes than equations which only predict a general trophic state, i.e., the equations developed above or the Vollenweider relationship mentioned below.[26]

Dillon posited that summer chlorophyll a concentrations in a lake were highly correlated with phosphorus, P, loadings to the lake during the spring. Chlorophyll a is a green, light-trapping pigment which is essential in the process of photosynthesis and is therefore an indicator of algal productivity and biomass, and hence a measure of eutrophication. Using regression analysis, Dillon developed a statistical NSM from cross-sectional data for a large number of lakes. The result of Dillon's analysis is a regression equation which relates the log of summer chlorophyll a concentration to the log of mean phosphorus loading in the spring. The derived equation was: log (chlorophyll a) = 1.5 log (P) - 1.1 , where chlorophyll a is the mean summer concentration, milligrams/m^3 of lake volume, and P is the spring mean phosphorus loading, milligrams/m^3 of lake volume. Figure 4-8 shows this log-linear relationship.

Figure 4-8. Relationship between Summer Chlorophyll a Concentration and Spring Phosphorus Loading



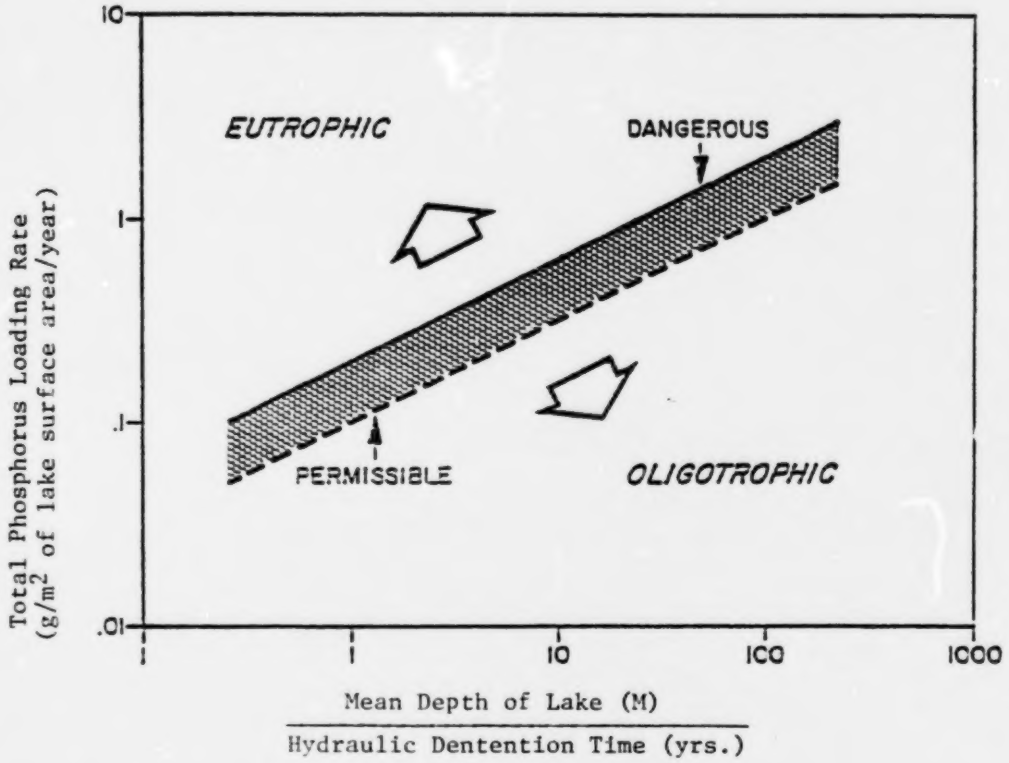
Source: Figure modified from Stanley W. Zison, Kendall F. Haven, and William B. Mills, Water Quality Assessment, Report No. EPA-600/9-77-023, prepared for Environmental Protection Agency (Lafayette, Calif., Tetra Tech, Inc., 1977) figure V-25, p. 343.

Accepting that mean summer chlorophyll a concentration is indicative of the level of eutrophication, this relationship can be used for any lake with characteristics similar to those in Dillon's sample. Given an estimate of the spring mean phosphorus loading for a lake, a crude estimate of mean summer chlorophyll a concentration can be made.[27]

The Vollenweider relationship, discussed in Zison, et al. (1978), predicts only whether a lake is eutrophic or is in danger of becoming eutrophic or oligotrophic, based on P_r, the phosphorus loading rate, grams/square meter of lake surface area per year, and Q_s, the mean depth of the lake, meters, divided by the hydraulic detention time, years. Vollenweider developed this relationship by plotting P_r and Q_s values for various lakes and making observations as to the eutrophic state of each lake. The Vollenweider relationship, shown in figure 4-9, does not produce a prediction of ambient concentration. Therefore it is not a statistical NSM, by definition.

It is important to emphasize that both the Dillon model and the Vollenweider relationship assume a priori that phosphorus is the limiting nutrient in the eutrophication process, while Shannon and Brezonik make no such assumption. Although it has been shown that phosphorus is the limiting nutrient in most lakes, this is not always the case. Therefore, in order to use either the Dillon model or the Vollenweider relationship, it must first be determined that the lake to be analyzed with respect to eutrophication is phosphorus-limited.

Figure 4-9. The Vollenweider Relationship



Source: Figure modified from Stanley W. Zison, Kendall F. Haven, and William B. Mills, Water Quality Assessment, Report No. EPA-600/9-77-023, prepared for Environmental Protection Agency (Lafayette, Calif.,Tetra Tech., Inc., 1977) figure V-23, p. 336.

Summary Comments

The preceding examples have briefly illustrated how statistical NSMs for analyzing receiving waters are derived and applied. Limitations of NSMs based on the statistical approach have been discussed in chapter 2 and briefly touched on again in this discussion. Despite these limitations, NSMs based on the statistical approach can be useful in certain receiving water problem contexts, as the work of Shannon and Brezonik demonstrates.

All of the examples presented underline the uncertainty relating to both the variables in, and the form of, relationships which can be used to predict the physical phenomena of interest in a statistical NSM.[28] In two of the four examples--Kelch and Lee, Shannon and Brezonik--the way in which the modelers went about identifying the form of the relationship is described. In summary, they experimented. Kelch and Lee were concerned with identifying the most important variables affecting the relationship, whereas Shannon and Brezonik believed that they knew the important variables and hence needed only to discover the relationship among them which best predicted the dependent variable. Although not described, the modelers in the other two examples also went through similar manipulations to arrive at the relationships they finally used. The point is that because of the nature of statistical tools, i.e., treating the natural system being analyzed as a black box, the procedure is simply to search out variables and relationships based primarily on the criterion of best statistical fit. Herein lies a major potential danger. Regardless of the goodness of the statistical fit, unless the relationship(s) derived are explainable in relation to the phenomena they seek to represent, they are likely to provide little or no information of use in analysis for REQM.

SELECTING AN APPROPRIATE RECEIVING WATER NSM

This section has two purposes. The first is to assist an REQM analyst in determining whether or not the proposed receiving water analysis is feasible. The second is to assist in the selection of an NSM which is the best suited for the application based on other relevant criteria.

The section corresponds to the section on setting up the natural systems analysis in chapter 2. Chapter 2 indicated a logical sequence of steps which could be followed to ascertain what type of natural systems analysis to undertake in any given context. Six steps were identified and described in table 2-3. The fourth step in the sequence related to determining the feasibility of carrying out the natural systems analysis specified in the previous three steps; the fifth step related to selecting an NSM for application based on relevant evaluation criteria. The material in this section is therefore an extension of these two steps, given a context in which analysis of one or more receiving water bodies is required.

Five elements comprise the section: (1) a listing of a number of receiving water NSMs, both operational and nonoperational, known as the population table; (2) a table which relates receiving water problem characteristics to the operational NSMs in the population table, referred to as the problem table; (3) a flow diagram which indicates how to select an appropriate receiving water NSM using the material included in the chapter, referred to as a selection procedure; (4) a discussion of the characteristics which are used to summarize each of the operational receiving water NSMs, referred to as model characteristics; and (5) summaries of the characteristics of the operational receiving water NSMs, referred to as model summary tables. Model summary tables for 27 receiving water NSMs are contained in Appendix A to the chapter.

Population of Receiving Water Models

Table 4-2 lists the receiving water models which were reviewed in preparing this chapter. This compilation comprises only NSMs based on the conservation of mass and energy approach. It is fair to say, however, that the majority of receiving water NSMs currently in general use are represented in the population. In cases where a number of models were essentially the same,

Table 4-2. Population of Mathematical Models of Receiving Waters for Potential Application in REQM Analysis

Model Category/Model Name	Commonly Used Acronym	Originator
Conservation of Mass Approach		
● Chemical Reaction Models		
Analytically Integrated		
Streeter-Phelps Dissolved Oxygen Equation	---	Indiana State Board of Health, Bloomington, Indiana
Lumped Parameter Nutrient Budget Model	---	Center for Inland Waters, Canadian Fisheries Research Board, Burlington, Ontario
Long Term Phosphorus Balance Model	---	Battelle Pacific Northwest Labs, Richland, Washington
Segmented River Dissolved Oxygen Model	---	Manhattan College, New York, New York
Steady-State Stream Network Model	SNSIM	U.S. Environmental Protection Agency-Region II, New York, New York
Simplified Stream Model*	SSM	Hydroscience, Inc., Westwood, New Jersey
Simplified Estuary Model*	SEM	Hydroscience, Inc., Westwood, New Jersey
Numerically Integrated		
Dissolved Oxygen Sag Model*	DOSAG-I	Texas Water Development Board, Austin, Texas
Dissolved Oxygen Sag Model* (revised version)	DOSAG-3	Water Resources Engineers, Austin, Texas
River Basin Model	RIBAM	Raytheon Corp., Portsmouth, Rhode Island
SCI DOSAG Modification*	DOSCI	Systems Control, Inc., Palo Alto, Ca.
Estuary Model*	ES001	U.S. Environmental Protection Agency-Retion II, New York, New York
Automatic Quality Model	AUTO-QUAL	U.S. Environmental Protection Agency, Washington, D.C.
River Quality Model*	QUAL-I	Texas Water Development Board, Austin, Texas
Dynamic Estuary Model*	DEM	Water Resources Engineers, Walnut Creek, Ca.
Tidal Temperature Model*	TTM	U.S. Environmental Protection Agency, Pacific Northwest Laboratory, Corvallis, Oregon
Receiving Water Model Module of SWMM*[a]	RECEIV	Water Resources Engineers, Walnut Creek, Ca.
Receiving Water Model (modification)	RECEIV-II	Raytheon Corp., Portsmouth, Rhode Island
Receiving Water Model (modification)*	RIVSCI	Systems Control, Inc., Palo Alto, Ca.
Receiving Water Model (modification)*	WRECEV	Water Resources Engineers, Austin, Texas
Deep Reservoir Model*	DRM	Water Resources Engineers, Walnut Creek, Ca.
Lake Ecologic Model (modification of Deep Reservoir Model)*	LAKSCI	Systems Control, Inc., Palo Alto, Ca.
Reservoir Water Quality Model*	EPARES	Water Resources Engineers, Austin, Texas
Hydrocomp Hydrologic Simulation Program*	HSP	Hydrocomp, Inc., Palo Alto, Ca.
Water Quality Feedback Model (HAR03 modification)	FEDBAK03	U.S. Environmental Protection Agency-Region II, New York, New York
Coastal Circulation and Dispersion Model*	CAFE/DISPER	Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Mass.
Estuary Water Quality Model*	EXPLORE-I	Battelle Pacific Northwest Labs, Richland, Washington

Table 4-2. Population of Mathematical Models of Receiving Waters for Potential Application in REQM Analysis (Continued)

Model Category/Model Name	Commonly Used Acronym	Originator
● Chemical Reaction Models (continued)		
Nutrient Accumulation Model	SPLOTCH	U.S. Environmnetal Protection Agency, Rochester, New York
Coastal Water Quality Simulation Model	---	The New York City Rand Institute, New York, New York
MIT Lake Temperature Model	---	Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Mass.
Two-dimensional Stream Mixing Model	---	Water Resources Division, U.S. Geological Survey, Washington, D.C.
Pascagoula Estuary Model	---	Dept. of Civil Engineering, Mississippi State University, Mississippi
Estuarial Sediment Transport Model	SED-II	Dept. of Civil Engineering, University of California, Davis, Ca.
Outfall Plume Model*	PLUME	U.S. Environmental Protection Agency, Pacific Northwest Laboratory, Corvallis, Oregon
Transient Water Quality Network Model	---	Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Mass.
Willamette River Model	WIRQAS	Water Resources Division, U.S. Geological Survey, Washington, D.C.
Estuary Hydrodynamic/Salinity Model*	HYD/SAL	Texas Water Development Board, Austin, Texas
● Ecologic Models (All Numerically Integrated)		
River Quality Model (QUAL-I modification)*	QUAL-II	Water Resources Engineers, Walnut Creek, Ca.
Lake Ecologic Model (DRM modification)*	LAKECO	Water Resources Engineers, Walnut Creek, Ca.
Lake Ecologic Model (DRM modification)	EPAECO	Water Resources Engineers, Austin, Texas
Delaware River Ecologic Model	---	Resources for the Future, Inc., Washington, D.C.
Estuary Ecologic Model*	ECOMOD	U.S. Environmental Protection Agency, Washington, D.C.
Finite Element Estuary Ecologic Model	ECOFEM	Water Resources Engineers, Walnut Creek, Ca.
Finite Element Ecologic Model	TRANS II	Resource Management Associates, Lafayette, Ca.
Estuarine Aquatic Ecologic Model*	ESTECO	Texas Water Development Board/Water Resources Engineers, Austin, Texas
Lake Phytoplankton Model*	LAKE-1	Department of Civil Engineering, Manhattan College, New York, New York
Eutrophic Lake Quality Model	---	Battelle Pacific Northwest Labs, Richland, Washington
Lake Ecologic Model	CLEAN-CLEANER	International Biological Program, Lake George Project, Rensselaer Polytechnic Institute, New York
Water Quality in River-Reservoir Systems*	WQRRS	U.S. Army Corps of Engineers, Hydrologic Engineering Center, Davis, Ca.
Narragansett Bay Hydrodynamic Model*	---	Department of Ocean Engineering, University of Rhode Island, Narragansett, Rhode Island

Note: For references for models shown, see Appendix B at end of chapter. Asterisk (*) indicates that a model summary table has been prepared for this model. Information in addition to that found in the individual summary table can be found in the associated references listed in Appendix B.

[a] See table 3-1, chapter 3.

only one or two models were included as representatives of a "generic class" of models. Several comments concerning the population are warranted.

First, as indicated in chapter 2, in order for a model to be considered a receiving water model in this report, it must be capable of estimating temporal and spatial patterns of ambient water quality resulting from residuals discharges. Therefore, models solely concerned with the movement of water, i.e., hydraulic models representing building block 1 in figure 4-3, have not been included. However, because hydraulic models of one form or another are part of most receiving water NSMs based on conservation of mass and energy, they are implicitly included in the population.

Second, because of their limited applicability in most REQM contexts, physical scale models have not been considered and hence do not appear in the population, although physical scale modeling has had a long history of use in water resources planning, and in some contexts would be preferred to the models presented herein.[29]

Third, no receiving water NSMs based on the statistical approach have been included in the population. As indicated, receiving water NSMs based on the statistical approach are primarily used for first cut or preliminary screening purposes. As such, these NSMs represent simplified methods for analyzing receiving water bodies, as is clear from the illustrations presented earlier. References on both receiving water NSMs based on the statistical approach and simplified methods are contained in the appendix to chapter 2.

Fourth, receiving water NSMs based on the conservation of mass and energy approach which are comprised of only hydraulic and transport components--building blocks 1 and 2 in figure 4-3--and can deal only with conservative substances, are also not included in the population. However, several of the models included in the population can analyze many of the problems addressed by models comprised of only hydraulic and transport components, and can analyze additional problems as well. Typical problems addressed by models based solely on hydraulic and transport components include: sediment deposition in reservoirs; sediment movement--including bedloads--in water bodies of all types; transport of dissolved solids in flowing streams and rivers; and flood routing. Information on models which address these types of problems only--transport of water and conservative substances--can be found in such sources as ASCE (1973), ASCE (1975), and ASCE (1976).

Fifth, the receiving water models compiled in table 4-2 are models which are comprised of either: (1) hydraulic, transport, and chemical reaction components--building blocks 1, 2, and 3 in figure 4-3--and identified as "chemical reaction models" in the table; or (2) hydraulic, transport, chemical reaction, and ecologic components--all 4 building blocks in figure 4-3--and identified as "ecologic models" in the table. The models listed under chemical reaction in table 4-2 are further disaggregated under the subheadings "analytically integrated" and "numerically integrated." This disaggregation separates the models as to complexity. NSMs which are numerically integrated are considerably more complex than those integrated analytically. All of the models listed under ecologic are numerically integrated.

In total, 50 receiving water models are listed in table 4-2. From this population, detailed summaries were made of 27 models defined to be operational. These are identified on table 4-2 with asterisks. As defined previously, to be operational an NSM must have two attributes. One, it must have been successfully applied to, and verified for, at least one application and can be used to model another roughly similar water body without extensive internal modifications. Two, sufficient written documentation must be available about the model to enable a user to apply the model in a location other than that for which it has been verified.

Relating Problems to Operational Models

Table 4-3 relates the 27 operational receiving water models identified in the previous section to the major receiving water problems discussed in the first section of the chapter. The purpose of this table is to provide an efficient manner in which to review the capabilities of the operational models in terms of typical problems which are likely to be encountered in different types of water bodies under varied flow conditions, for any given REQM analysis.

In the table, each of the seven major problems--temperature, salinity, erosion and sedimentation, dissolved oxygen, eutrophication, toxic substances, and biological effects--has been further subdivided into subheadings. The subheadings enable more detailed distinctions to be made among the capabilities of various models. The seven major problems and the subheadings within each represent most of the water quality problems which will be encountered.

Based on this table, a analyst can develop two sets of information. One, for any given set of problems or problem aspects, a number of operational models which can deal with these problems can be identified. Two, for any given operational model identified in the table, the problems that it can address can easily be identified, and other models capable of addres-

Table 6-3. Receiving Water Models and Their Relevance to Specific Problems

MODEL	WATER BODY CHARACTERISTICS										MAJOR PROBLEMS																									
	WATER BODY TYPE					FLOW CONDITIONS					TEMPERATURE			SALINITY				EROSION & SEDIMENTATION			DISSOLVED OXYGEN				EUTROPHICATION			TOXIC SUBSTANCES				BIOLOGICAL EFFECTS				
	Streams	Rivers	Lakes	Estuaries	Offshore Waters	Constant Streamflow	Variable Streamflow	Tidal Action	Steady State Lake Levels	Variable Lake Levels	Ambient Variations	Waste Heat Inputs	Thermal Stratification	Natural Salt Sources	Irrigation Return Flows	Saltwater Intrusion	Salinity Stratification	Bedload Transport	Suspended Solids Transport	Absorbed Residuals Transport	Carbonaceous Oxygen Demand Nonpoint Sources	Carbonaceous Oxygen Demand Point Sources	Nitrogenous Oxygen Demand	Instream Oxygen Demand	Nitrogen Kinetics	Phosphorus Kinetics	Minor Nutrients	Heavy Metals	Pesticides	Refractory/Synthetic Organics	Radioactive Material	Decomposers Inc. Coliforms	Primary Producers	Zooplankton-Invertebrates	Fishes	Ecosystem-Level Indicators
SSM	●	●	●			●															●	●														
SKM		●		●		●										●					●	●														
DOSAG-I	●	●				●															●	●	●													
DOSAG-3	●	●				●								●	●						●	●	●		●	●		●				●	●			
DOSCI	●	●				●								●	●						●	●	●		●	●		●				●	●			
ES001				●		●		●								●					●	●		●								●	●			
QUAL-I	●	●				●															●	●	●									●				
DEM	●	●		●		●	●	●			●	●				●			●	●	●	●	●		●	●	●	●	●	*	*	●	●			
TTM	●	●		●		●	●	●			●	●				●																				
RECEIV	●	●	●	●		●	●	●	●	●						●					●	●	●		●	●	●	●	●	●	●	●				
RIVSCI	●	●		●		●	●	●			●	●				●					●	●	●		●	●	●	●				●	●			
WRECEV	●	●		●		●	●	●								●					●	●	●		●	●	●	●	●	*	*	●				
DRM			●			●	●		●	●	●		●																							
LAKSCI			●			●			●				●			●					●	●	●					●								
EPARES			●			●	●		●	●	●	●	●	●	●	●	●				●	●	●		●	●	●	●				●	●			
HSP	●	●	●			●	●		●	●	●	●	●			●					●	●	●		●	●	●	●	●	*	*	●	●	●		
CAFE/DISPER		●	●	●	●		●	●											○						○	○	○	○	○	○	○	○	○	○	○	
EXPLORE-I		●		●		●		●								●			●		●	●	●	●	●	●		●		●		●	●			
PLUME			●	●	●																	●														
HYD/SAL				●	●	●	●	●								●																				
QUAL-II	●	●				●					●	●		●	●				●		●	●	●		●	●		●	●	*	*	●	●			
LAKECO			●			●	●		●	●	●	●	●								●	●	●	●	●	●	●	●	●	●	●	●	●	●	●	
ECOMOD				●		●	●	●								●			●	●	●	●	●	●	●	●	●					●	●	●	●	
ESTECO				●	●	●	●	●								●				●	●	●	●	●	●	●	●					●	●	●	●	●
LAKE-I			●						●				●												●	●							●	●	●	
WQRRS	●	●	●			●	●		●	●	●	●	●	●	●	●	●		●		●	●	●	●	●	●	●					●	●	●	●	
Narragansett Bay Model				●	●	●	●	●			●					●					●	●	●		●	●							●	●	●	

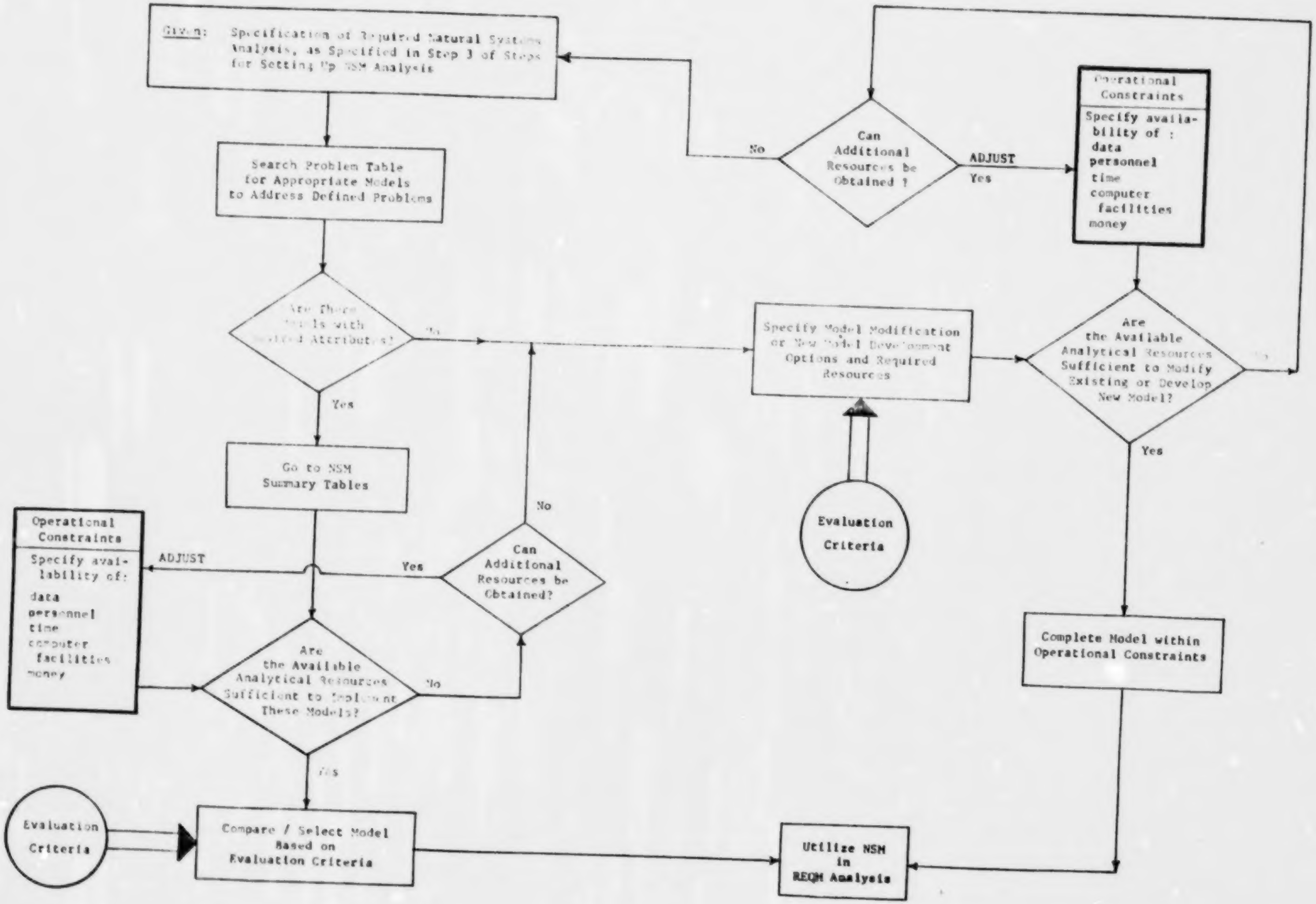
● applicable ;   ○ applicable if treated as discrete particles ;   * applicable if treated as conservative constituent sing the same problems identified. Although problems which models address can be identified using the table, no information can be obtained from the table as to how and with what level of specificity a model can analyze a given problem. Therefore, table 4-3 must be used in conjunction with the model summary tables in Appendix A. Given a number of models of interest identified by means of table 4-3, the model summaries in Appendix A then provide the requisite details about each model. Both table 4-3 and the model summary tables are integral parts of the procedure for selecting a receiving water model.

Procedure for Selecting a Receiving Water NSM

The procedure for selecting a receiving water NSM is directly tied to steps 4 and 5 in the section on setting up the natural systems analysis in chapter 2. Given that the natural systems analysis required in a given REQM analysis has been specified in terms of one or more receiving water bodies to be analyzed, the analyst would then follow the procedure contained herein to select an appropriate receiving water model. The procedure indicates the questions which must be asked and the activities undertaken before an appropriate model can be selected, given operational constraints. Further, the procedure is the vehicle which operationally integrates the various sections of this chapter. Figure 4-10 represents the procedure for selecting an appropriate receiving water model. Note that the procedure is identical to the flow chart of the NSM selection process contained in figure 2-6 of chapter 2. This is not the case for all categories of NSM models.

Given that the required natural systems analysis has been specified, the procedure begins with a search of the problem table. If one or more candidate models are identified in the table, the analyst then goes to the

Figure 4-10. Procedure for Selecting a Receiving Water Model


Given: Specification of Required Natural Systems Analysis, as Specified in Step 3 of Steps for Setting Up NSM Analysis
Search Problem Table for Appropriate Models to Address Defined Problems
Are There Models with Desired Attributes?
No
Yes
Go to NSM Summary Tables
Operational Constraints
Specify availability of:
data
personnel
time
computer facilities
money
ADJUST
Yes
Can Additional Resources be Obtained?
No
Are the Available Analytical Resources Sufficient to Implement These Models?
No
Yes
Evaluation Criteria
Compare / Select Model Based on Evaluation Criteria
Utilize NSM in REQM Analysis
Specify Model Modification or New Model Development Options and Required Resources
Evaluation Criteria
Can Additional Resources be Obtained ?
No
ADJUST
Yes
Operational Constraints
Specify availability of :
data
personnel
time
computer facilities
money
Are the Available Analytical Resources Sufficient to Modify Existing or Develop New Model?
No
Yes
Complete Model within Operational Constraints

summary tables to obtain and tabulate the relevant information for each of the candidate models. Table 4-4, the model summary table prepared for the DOSAG-3 Model developed by Water Resources Engineers, illustrates the format for, and types of information in, the summary tables. Descriptions of the characteristics of this table pertaining to all NSMs were in chapter 2. Additional points relating to those characteristics in relation to receiving water NSMs and descriptions of characteristics applicable solely to receiving water NSMs are contained in the next section.

Next, the available analytical resources to utilize the models are compared with the resources required. If several models can be applied within the operational constraints, then a model is selected on the basis of the evaluation criteria discussed in chapter 2. If only one model can be applied within the operational constraints, then that model would be chosen, unless it did not meet some evaluation criterion deemed critically important.

If no candidate model can be applied within the operational constraints, the logical first option is to attempt to increase the available analytical resources to the level equal to those required to apply at least one of the candidate models. If the additional resources cannot be obtained or if no models can be located in the problem table which are capable of addressing the problems of concern, the analyst has three choices. First, the literature can be searched to locate operational models not included in the table which will satisfy the analysis requirements. Of course, in order to choose among any additional models discovered--in relation to operational constraints and the evaluation criteria--information comparable to that contained in the model summary tables in Appendix A is required. Second, modifications could be made to an existing model to satisfy analytical specifications, given operational constraints and the evaluation criteria. Third,

Table 4-4. Summary of the Revised Dissolved Oxygen Sag Model (DOSAG-3)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Water conveyance canals
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal variation only; (3) Morphology: (a) DOSAG-3 permits no stratification (each reach well-mixed), (b) branched watershed network can be simulated
Time Properties	(1) Time variability: (a) steady state; (2) Time units of application: (a) variable depending upon total length of the system and prescribed flow
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) up to 49 stretches, (b) maximum of 80 reaches, (c) maximum of 20 headwaters, (d) up to 20 reaches per stretch
Physical Processes	(1) Principal driving force: (a) net downstream flow; (2) Processes represented: (a) advection, (b) dilution
Chemical Processes	(1) Processes represented: (a) chemical interactions, both coupled and uncoupled; (2) Constituents modeled: (a) dissolved oxygen, (b) carbonaceous BOD, (c) nitrogenous BOD, (d) phosphorus, (e) ammonia, (f) nitrite, (g) nitrate, (h) conservative materials--total N, chlorides, metal ions, e.g., iron
Ecological Processes	(1) Processes represented: (a) photosynthesis, represented by chlorophyll A, (b) coliform die-off, (c) first order bacterial decay, (d) algal respiration; (2) Trophic levels: (a) only decomposers and primary producers simulated; (3) Water quality-biota relationships represented: (a) algal (chlorophyll A)/nutrient dynamics
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) analytical integration (Laplace transforms), (b) utilizes LaGrangian approach where computations performed on reach by reach basis (progressing downstream)
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 27,000 word storage capacity, (b) FORTRAN IV compiler, (c) no disks or tapes
Input Data Requirements	(1) Initial setup/calibration: (a) reach length, (b) mean discharge, (c) mean reach velocity, (d) mean reach depth, (e) average reach temperature, (f) residuals discharge inflows, (g) withdrawals and groundwater inflows, (h) constituent concentrations in all inflows, (i) initial constituent concentrations by reach; (2) Verification: (a) observed streamflow, (b) observed stream velocities, (c) observed constituent concentrations throughout the modeled area
Ease of Application	(1) Model documentation: (a) documentation report available from EPA, Systems Development Branch, Washington, D.C.; (2) Documentation contents: (a) complete documentation contains theory, subroutine descriptions, file and data deck design, program listings, and sample problem; (3) Modifications: (a) little recomputation time needed for data deck changes
Output and Output Format	(1) Output information: (a) constituent concentrations in each reach, (b) flow rate, (c) reach depth, (d) minimum dissolved oxygen value and river mile where it occurs, (e) mean velocity, (f) algae growth rate; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Model cannot handle nonpoint residuals discharges except as tributary inputs (incremental runoff inputs)
Manpower Needs	(1) Requires one junior-level engineer with some basic programming experience
Costs	(1) Model acquisition: (a) documentation reports may be obtained for a nominal charge from EPA, Washington, D.C. or Water Resources Engineers, Austin, Texas; (2) Model setup and data preparation: (a) requires 2-7 man-weeks; (3) Actual computation: (a) $2-8 per simulation run; (4) Output analysis: (a) small, e.g., less than one hour
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes constant stream velocity throughout a reach, (b) assumes first order decay only; (2) Sensitivity: (a) high sensitivity to residuals inputs, stream velocities, (b) moderate sensitivity to flow and decay coefficients
Other Comments	(1) Limitations: (a) DOSAG-3 cannot compute nitrogenous BOD and other nitrogen species (ammonia, nitrite, nitrate) simultaneously; (2) Optional features: (a) flow augmentation option to reach prescribed DO standards, (b) model permits three different treatment efficiencies for residuals discharges; (3) DOSAG-3 derived from DOSAG-I by Water Resources Engineers, Austin, Texas

[a] Also included in Appendix A as table 4A-4.

a new model could be developed from "scratch." The second and third choices are shown in the procedure; the first is not. The possibility will always exist that there are models in the literature heretofore passed over which, when investigated, could be suitable in a given context. If one, two, or three cannot be accomplished due to operational constraints, the evaluation criteria, or lack of knowledge, then the required receiving water analysis, i.e., questions to be answered, must be respecified and the procedure repeated.

Developing a new model from scratch entails basic theoretical mathematical formulation, debugging after initial set up, sensitivity testing, calibration, and verification. These together represent a level of effort considerably above that involved in applying an existing operational model. Model development requires certain specialized technical skills and substantial resources. It should be undertaken in an REQM analysis only after very careful consideration.

Finally, the procedure described above should not be viewed only in terms of the information presented in this chapter and its appendix. The activities and questions identified in the procedure are relevant for selecting a receiving water NSM under any analytical conditions.

Discussion of Characteristics Used to Summarize Receiving Water Models

Table 4-4 illustrates the way in which operational receiving water models are summarized in Appendix A. Seventeen characteristics are shown for which information on operational receiving water models is provided, information which is important to know in order to select an appropriate model in a given context. Chapter 2 contained descriptions of nine of these characteristics relevant to all categories of NSMs: computational status, input data requirements, ease of application, output and output format, linkages to other models, manpower needs, costs, model accuracy and sensitivity, and other comments. The remaining eight characteristics are discussed here. Also, where relevant to receiving water models, some specific comments are made about the characteristics discussed in chapter 2.

Applicable Receiving Water Body

The types of receiving water bodies for which models are available include streams, rivers, lakes, estuaries, coastal and off-shore waters, and man-made conveyance systems. Although some models are very site-specific, pertaining only to a certain type of water body or set of water bodies with similar features, others can be applied to different types of water bodies with few modifications.

Water Body Characteristics

Water body characteristics identify additional features about the water bodies to which a receiving water model can be applied. Identifying just the type of water body to which a model may be applied is, by itself, insufficient for ascertaining model applicability for a given REQM analysis. Important additional characteristics include scale, areal boundaries, and hydrogeomorphological features.

Scale relates to the size of the water body or bodies to which a model is applicable. In this regard receiving water models have been identified as either near field or far field models. Near field models are those used in relation to site-specific analyses, for example, analyzing the effluent stream(s) from a given activity such as a power plant or a refinery. Near field models deal with relatively small sections of receiving water bodies and typically consider advection and diffusion as the primary processes affecting ambient concentrations. Because of the relatively small scale, transformations of residuals by other physical processes and chemical and biological processes are often assumed to be negligible. Far field models are applicable to entire water bodies, such as an estuary, or to large sections of water bodies, e.g., a specified area of coastal off-shore waters. In far field models, site specific features such as discharge plumes from individual activities cannot be distinguished. Most far field models assume that residuals discharges are uniformly mixed within the individual segments into which a water body is divided for analysis, e.g., a river reach.

Areal boundaries relate to the latitudinal and longitudinal boundaries of water body systems which a model can incorporate. For example, can a model consider stratification in a water body? In an off-shore marine system, can a model consider both deep portions of the system and shallow areas close to shore? The processes affecting the movement of water in off-shore areas are different from those affecting movement in shallow in-shore areas, hence the related mathematical formulations differ.

Flow conditions and hydrogeomorphological features are two of the most important water body characteristics about which a model's capability to represent should be known. Types of flow conditions include continuous steady flows (constant), nonsteady flows (variable), and intermittently variable flows, i.e., because of runoff. In many cases, flow conditions can serve as a useful factor for comparing models, because the ability to analyze different flow conditions indicates different capabilities with respect to modeling hydraulic processes and transport phenomena. Hydrogeomorphological features are closely related to flow conditions because they affect the movement of water within a water body. Hydrogeomorphological variables of importance include depth, composition of bottom strata, watershed size, and gradient of the water body.

Time Properties

Receiving water models differ in the way in which they consider time-dependent variables, particularly flow conditions, residuals discharge inputs, and meteorological conditions. As indicated in chapter 2, NSMs can be grouped into three categories according to time properties: steady state, quasi-nonsteady state (referred to as quasi-steady state on model summary tables), and nonsteady state. Definitions of these categories were given in chapter 2.

In steady-state receiving water models, residuals discharge inputs, flow conditions, and meteorologic conditions such as temperature, precipitation, and wind, are held constant. Under these conditions ambient concentrations of residuals are a function of advection, diffusion, and constant transformation rates for the material or energy residuals. In quasi-nonsteady-state receiving water models, meteorologic conditions are permitted to vary with time, thereby altering certain transformation rates, e.g., biological decomposition and aeration, over time. Residuals discharges and flow conditions are held constant. In both steady-state and quasi-nonsteady-state receiving water models, impacts of alternative flow conditions and residuals discharge inputs can be determined only by rerunning the model with different sets of each. Nonsteady-state receiving water models permit flow conditions, residuals discharge inputs, and meteorological conditions, all to vary with time. Depending on the problem context, models with different time properties will be more or less applicable, and necessary, to answer the specified questions.

Another important time property consists of the time units of application. Time units of application refer to: the averaging time or times permissible in a model (also referred to as time steps), and the time period over which a model can be run. For example, a nonsteady-state receiving water model could be run over a time period of several days with an averaging time or time step of one hour. In this case, estimates of ambient concentrations would be made for every hour for several days.

Space Properties

Spatial properties of receiving water models include the dimensionality and discretization features of the model. Spatial dimensionality relates to the number of dimensions which a model can represent. Spatial dimensionality is relevant to spatial patterns of residuals concentration which can be estimated. For example, a three-dimensional model--movement permitted in the x, y, and z dimensions--will enable predicting both vertical and horizontal variations in residuals concentrations. A two-dimensional model--varying in the x and y directions--usually assumes spatial homogeneity in the third dimension. When the spatial dimensions of a model are identified, it is also necessary to specify which geometric plane is being considered, i.e., vertical or horizontal. For example, a one-dimensional model can represent both river channels (linear systems) or stratified lakes (layered systems), but the lake model considers only vertical variations and the river model considers only horizontal variations.

It is important to understand the limitations of nonsteady state two- and three-dimensional receiving water models. First, no nonsteady-state three-dimensional models exist that can be considered totally operational, although some are under development. Thus, the analyst should not expect to find a receiving water NSM with that capability.

Second, although there are operational nonsteady state two-dimensional models, there are very few instances of successful verification of this type of model. Many current two-dimensional models are pseudo two-dimensional, consisting of a two-dimensional network of linked one-dimensional channels, for which accurate results often depend upon the method and degree of discretization. Verification of such models is tenuous at best. Certain vertically integrated, two-dimensional (horizontally) finite difference and finite element models are more readily verified, but even with these verification is very difficult. This discussion is intended to emphasize these difficulties so that the analyst will not expect more than is feasible from two-dimensional, nonsteady state receiving water models.

Discretization is the extent to which a model can divide a water body into functional volumes that can account for geographical and topographical variations. In riverine systems, the discretization procedure involves setting up linear river segments (reaches) with appropriate headwaters, tributary branches, and river confluences (junctions). A reach might represent one or more river miles, depending upon the limitations of the model in relation to the prototype system's size and complexity. Deep water bodies that exhibit thermal or salinity-induced density stratification are often divided into separate layers. Large, well-mixed estuaries or lakes might be divided into equal-sized grids--perhaps one square mile or one square kilometer--to enable consideration of horizontal variations, as indicated in figure 2-2 in chapter 2.

Physical, Chemical, and Ecological Processes

These three characteristics are essentially discussed in the section entitled Major Natural Processes. However, two points merit discussion here:

one in relation to how receiving water models consider temperature, the other with respect to chemical reactions.

Temperature measures the amount of heat within a mass of water and can be represented to varying degrees in receiving water models. Certain models treat temperature as a specific variable that must be evaluated, i.e., as a total heat (energy) budget within the water body. Other models use temperature only to adjust particular process rates. (Ambient temperature directly affects the physical state of water, reaeration rates, and reaction rates in chemical and biochemical processes.) Further, some models do not consider actual temperature variation in the modeled water body except that water masses with different temperature characteristics are treated as separate entities, such as different lake layers. Still other receiving water models deal exclusively with system hydrodynamics and associated heat budgets to simulate temperature profiles.

In the model summary tables, chemical reactions are characterized as either coupled or noncoupled. Chemical reactions between or involving different materials are termed coupled reactions. Because the mass balance for each material depends on the presence or behavior of other materials, interconnected equation sets are necessary. Coupled reactions usually have a source or sink term connected directly to a separate chemical reaction. For example, the chemical transformations (oxidation) of nitrogen among its various aqueous forms (ammonia, nitrite, and nitrate) depend on the presence of dissolved oxygen. Noncoupled chemical reactions describe conversions that are independent of other materials and their chemical reactions. A residual which undergoes settling, degradation, or specific conversions that do not involve other chemical materials belongs in the noncoupled reaction category. Total dissolved solids or inert sedimentary particles are materials whose transformations are typically represented by non-coupled reactions.

Mathematical Properties

Two types of mathematical properties of a receiving water model are important to identify: one, the theoretical mathematical basis; and two, the solution technique used to solve the equations in a model. The important distinction to identify regarding the theoretical mathematical basis is whether a model is stochastic or nonstochastic (deterministic). Most receiving water models combine both approaches, for example, models which permit variable stormwater input flows.

All of the models included in Appendix A are solved using either analytical or numerical integration solution techniques. The techniques employed are indicated under this characteristic and chapter 2 discusses these solution techniques in general.

Output and Output Format

Generally, the output of a receiving water model consists of the spatial and temporal distribution of residuals concentraitons or AEQ indicators throughout a receiving water body. Typical output data produced by a receiving water model include flow velocities, stage height, residuals concentrations or values for AEQ indicators, at various spatial locations for selected averaging times. Water quality indicators, for example, are most frequently described in terms of concentrations, milligrams per liter.

Ambient water quality indicators can be reported at preset points, e.g., average concentrations per stream reach or at each junction in a link-node grid, or user-selected points within the original discretization format, depending on the model. In finite element models, output values describing flow might be presented in terms of current vectors. Output values are also frequently provided at major model boundary points, because such points represent shoreline, seaward, or downstream edges of a modeled receiving water body. These boundary values are especially important when simulating several different, but interconnected, water bodies at the same time, or when the output from one region is the input to a different region. When using certain types of grid format, model output for certain variables is presented as areal averages, such as kilograms per hectare or number per square meter.

Linkages to Other Models

Because no receiving water model NSM is applied in a vacuum, it is important to indicate how a given model can relate to other segments of an REQM analysis. Whenever possible, consideration should be given to selecting a receiving water model which predicts changes in water quality indicators that can be related to perceived damages. For example, when a reduction in sport fishing, commercial fishing, or both is identified as a "major" damage resulting from residuals discharges, e.g., decreased bluefish catch or clam harvest in the Chesapeake Bay region, the receiving water model selected for application should be capable of predicting impacts on the particular species of concern.

Another type of linkage is the compatibility of a receiving water model with respect to other natural systems models. In many REQM contexts, more than one natural systems model will be employed; in some contexts more than one receiving water model. An example of the former is a context in which urban or nonurban runoff models are used to estimate residuals discharges to a receiving water body, a water body which potentially is to be analyzed using a particular receiving water model. An example of the latter is a context in which different parts of an interconnected water body system, e.g., composed of lakes and rivers, are analyzed using different models. In such a case, the outputs of one model, i.e., at its boundaries, would provide inputs into another; therefore the models must be consistent with each other.

Concluding Comment on Model Selection

The foregoing discussion has shown the requisite steps for choosing a receiving water model for a given application. The procedure is applicable regardless of the context. The characteristics which have been chosen to summarize the receiving water models contained in Appendix A are useful as a "blueprint" for all receiving water models. As additional models become operational, they can be summarized in the format presented herein and added to Appendix A.

Germane to any discussion of model selection is identification of the problems which relate to model application. An understanding of these problems enables more intelligent use to be made of the available material on NSMs, included in this report and elsewhere, for selecting an appropriate NSM. The last section in chapter 2 described the major problems relating to present applications of natural systems models. These problems are generally relevant for all categories of NSMs, and should be reviewed before making final model selections.

NOTES

[1] Surface receiving waters are referred to simply as receiving waters throughout the report.

[2] Thermal stratification is the separation of water into levels in natural lakes and man-made impoundments as a result of water density differences produced by temperature differences.

[3] Suspended solids is the more "generic" term, encompassing any solid material transported in suspension by water, including plastic, aluminum cans, tree limbs, tires, as well as soil particles.

[4] Information regarding the National Eutrophication Survey can be obtained from the Office of Water Planning and Standards of the U.S. Environmental Protection Agency, Washington, D.C.

[5] For a discussion of how toxic substances are presently identified, see Maugh (1978) and Culliton (1978).

[6] Biological effects are also sometimes referred to as ecological effects. These two terms have been used interchangeably, although this is not completely correct. For clarification, see the section on major processes.

[7] An autotrophic organism is an organism capable of constructing organic matter from inorganic substances.

[8] See table 2-1 in chapter 2.

[9] If residence time is sufficiently long, precipitation of dissolved salts can occur, e.g., as in some reservoirs.

[10] For a discussion of these processes, see Linsley, Kohler, and Paulhus (1949) and (1975).

[11] The documentation for many operational receiving water NSMs does not indicate how the hydraulic inputs can be obtained, but rather only the types of hydraulic inputs with which the model operates.

[12] The exceptions are those which employ measured data in conjunction with the continuity equation only.

[13] This derivation is taken from an unpublished paper by Walter O. Spofford, "Water Quality Modles--Past, Present, and Future," Resources for the Future, Washington, D.C., April 1972.

[14] The exact expression for this is: $\frac{\partial A}{\partial t} = b\,\frac{\partial h}{\partial t} + h\,\frac{\partial b}{\partial t}$. The derivation assumes that $\frac{\partial b}{\partial t} = 0$.

[15] These coefficients are discussed in chapter 2.

[16] For a complete definition of the advective-diffusion equation, see Daily and Harleman (1966).

[17] See chapter 2 for a discussion of this point.

[18] For additional explanation, see O'Connor (1967).

[19] For a survey of aquatic ecosystem models, see Parker and Roop (1974).

[20] Other statistical methods which have been used include Fourier series and power spectrum methods, e.g., by Thomann (1967) to analyze ambient dissolved oxygen concentrations and temperature in the Delaware estuary. Power spectrum methods were used by Wastler and Walter (1968) to analyze the relationship between freshwater inflow and ambient chloride concentrations in the Charleston, South Carolina harbor.

[21] Impoundments differ from lakes in that they are man-made, for example, a reservoir or man-make lake, and thus have slightly different characteristics from natural lakes. In such systems the amount of water residing in the impoundment is regulated over time by man, and bottom characteristics and sedimentation rates are also likely to differ from those of natural lakes. Aside from these aspects, analysis of impoundments is essentially the same as analysis of lakes.

[22] Given a multiple regression equation, a stepwise procedure performs iterations of the regression, sequentially either removing or adding specified independent variables to a regression equation based on a prespecified significance test. The final result of a stepwise procedure is an equation which is comprised of the independent variables which best explain the dependent variable--based on the coefficient of determination--given the prespecified level of significance.

[23] Kelch and Lee (1978) do not indicate the unit(s) for this variable, nor how it was measured. The paper describes how variables such as X_{48} and X_{94} were measured.

[24] For a description of how the nitrogen and phosphorus loadings and the trophic state index were actually computed, see Shannon and Brezonik (1972a and 1972b).

[25] Shannon and Brezonik also use canonical correlation to analyze relationships among the variables comprising the trophic state index, and the relationship between N and P loadings. Reporting this analysis is not necessary for illustrating the analytical approach employed.

[26] The Vollenweider relationship is perhaps the most widely used relationship to relate phosphorus loading to eutrophication. It is used in the National Eutrophication Study to assess the extent of eutrophication in United States' lakes. The Vollenweider relationship is described in Vollenweider (1975).

[27] The following points concerning the Dillon relationship are not specified in the source document (Zison, et al., 1978): the months comprising "summer" and "spring;" the basis of mean chlorophyll a concentration, e.g., mean of daily measurements or weekly measurement; how the total phosphorus load for the spring is derived; and whether or not washout of P from precipitation onto the lake surface is included.

[28] Specification is also a problem for NSMs based on conservation of mass and energy.

[29] Physical models, ranging in size from simple aquarium microcosms to the large-scale U.S. Army Corps of Engineers' models of Chesapeake Bay and San Francisco Bay, have been used to represent certain characteristics of water bodies in varying degrees of specificity. Physical models can readily simulate system hydraulics and transport of certain conservative substances, e.g., total dissolved solids. However, nonconservative materials which settle, adsorb, or transform chemically and biochemically, cannot be assumed to behave in physical models as in natural systems. Because each condition to be analyzed requires a separate application, and because the physical models' basic structure and initial conditions are typically site-specific, these models are heavily dependent upon prevailing operating conditions.

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Appendix A:

SUMMARY TABLES OF RECEIVING WATER MODELS

Table 4A-1. Summary of the Simplified Stream Model (SSM)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Shallow, non-stratified lakes
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) considers only longitudinal variations; (b) handles only point source residuals inputs
Time Properties	(1) Time variability: (a) steady-state
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane
Physical Processes	(1) Principal driving force: (a) net flow and velocity; (2) Processes represented: (a) dilution, (b) advection, (c) reaeration, (d) temperature effects
Chemical Processes	(1) Processes represented: (a) uncoupled chemical reactions, (b) coupled BOD-DO deficit; (2) Constituents represented: (a) BOD, (b) DO, (c) unspecified conservatives, (d) uncoupled non-conservatives with first order decay
Ecological Processes	(1) No biochemical processes represented directly, although first order decay for coliform bacteria possible.
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) solution of analytical equations by hand calculation or reference to nomograph charts provided in model handbook
Computation Status	(1) Model uncoded; (2) No computer equipment required except for an electronic hand calculator
Input Data Requirements	(1) Initial setup/calibration: (a) net river flow, (b) flow velocity, (c) depth, (d) distance from point source discharges, (e) constituent concentrations, temperature, and background DO deficit for all stream inflows, (f) loading rate for ultimate oxygen demand, (g) deoxygenation coefficients; (2) Verification: (a) constituent concentrations throughout the modeled area
Ease of Application	(1) Model documentation: (a) handbook available from EPA Planning Assistance Branch, Washington, D.C.; (2) Documentation contents: (a) adequate for most engineering applications, although examples of the required methodology are minimal; (3) Modifications: (a) recomputation time substantial because input changes require new solution of analytical equations
Output and Output Format	(1) Output information: (a) constituent concentrations, (b) DO deficit; (2) Output format: (a) hand calculations
Linkages to Other Models	(1) Output information is not used directly as input to other models, although model results may be used to develop more complex computer models
Manpower Needs	(1) Requires junior-level engineer or engineering aide with mathematical orientation; (2) No programming experience necessary
Costs	(1) Model acquisition: (a) nominal cost for handbook from EPA, or reproduction cost if original reports no longer available; (2) Model setup and data preparation: (a) may require 1-2 man-weeks; (3) Actual computation: (a) several man-hours to several man-days depending on the complexity of the application and mathematical skill of the personnel involved; (4) Output analysis: (a) small
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes constant stream velocity for each reach, (b) assumes first order decay rates for quality constituents; (2) Sensitivity: (a) high estimated sensitivity to residuals loading rates and stream velocities, (b) moderate estimated sensitivity to decay coefficients and total streamflow
Other Comments	(1) SSM developed by Hydroscience for EPA as a "first cut" planning tool, but its simplified nature restricts its usage when complicated prototype systems or complex water quality problems are involved; (2) SSM requires no computer programs to achieve reasonable "first cut" estimates of ambient DO downstream from point sources

Table 4A-2. Summary of the Simplified Estuary Model (SEM)

Characteristic	Summary Data
Applicable Water Body	(1) Tidal rivers; (2) Non-stratified estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) considers only longitudinal variations, (b) handles only point source residuals inputs
Time Properties	(1) Time variability: (a) steady state
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) No discretization limits
Physical Processes	(1) Principal driving forces: (a) net flow and velocity; (2) Processes represented: (a) advection, (b) longitudinal dispersion, (c) dilution, (d) reaeration, (e) temperature effects
Chemical Processes	(1) Processes represented: (a) uncoupled chemical reactions, (b) coupled BOD-DO deficit; (2) Constituents represented: (a) BOD, (b) DO, (c) unspecified conservatives, (d) uncoupled non-conservatives with first order decay, e.g., nutrients
Ecological Processes	(1) No biochemical processes represented directly, although first order decay for coliform bacteria possible
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) solution of analytical equations by hand calculations or reference to nomograph charts provided in model handbook
Computation Status	(1) Model uncoded; (2) No computer equipment required except for an electronic hand calculator
Input Data Requirements	(1) Initial setup/calibration: (a) net river flow exclusive of tidal effects, (b) flow velocities, (c) average depths, (d) distance from point source discharges, (e) dispersion coefficients, (f) cross-sectional area, (g) constituent concentrations, temperature and background DO deficit for all stream inflows, (h) loading rate for ultimate oxygen demand, (i) deoxygenation coefficients, (j) reaeration coefficients, (k) salinities at the seaward boundary; (2) Verification: (a) constituent concentrations throughout the modeled area
Ease of Application	(1) Model documentation: (a) handbook available from EPA Planning Assistance Branch, Washington, D.C.; (2) Documentation contents: (a) adequate, although examples of the necessary methodology for various applications are minimal, (b) good documentation summary can be helpful if time for model familiarization permitted; (3) Modifications: (a) recomputation time substantial because input changes require new solution of analytical equations
Output and Output Format	(1) Output information: (a) constituent concentrations, (b) maximum DO deficit, (c) minimum DO concentrations; (2) Output format: (a) hand calculations
Linkages to Other Models	(1) Output information is not used directly as input to other models
Manpower Needs	(1) Requires junior-level engineer or engineering aide with mathematical orientation; (2) No programming experience necessary
Costs	(1) Model acquisition: (a) nominal cost for handbook from EPA, or reproduction cost if original reports no longer available; (2) Model setup and data preparation, including model familiarization: (a) requires 1-2 man-weeks; (3) Actual computation: (a) several man-hours to several man-days depending on the complexity of the application and mathematical skill of the personnel involved; (4) Output analysis: (a) small
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes a constant velocity for each reach, (b) assumes first order decay rates for quality constituents; (2) Sensitivity: (a) moderate sensitivity (estimated) to residuals inputs, stream flow and velocity, and decay coefficients, (b) insensitive to dispersion coefficient
Other Comments	(1) SEM developed by Hydroscience, Inc. for EPA as a "first cut" water quality planning tool, but its simplified nature restricts its usage when complicated prototype systems or complex water quality problems are involved; (2) SEM requires no computer programs to achieve reasonable "first cut" estimates of ambient DO in estuaries downstream from point sources

Table 4A-3. Summary of the Dissolved Oxygen Sag Model (DOSAG-I)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Canals and other water conveyance systems
Water Body Characteristics	(1) Scale: (a) far field, (2) System boundaries: (a) longitudinal variation only; (3) Flows: (a) handles constant flows and inputs only
Time Properties	(1) Time variability: (a) steady state; (2) Time units of application: (a) time steps of one travel time through system utilized, (b) program requires one month run as minimum and 12 months as maximum, (c) daily averages given
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) 10 headwater stretches, (b) 20 junctions, (c) up to 50 reaches, (d) up to 20 stretches, (e) reach length variable, usually given in river miles
Physical Processes	(1) Principal driving force: (a) net downstream flow; (2) Processes represented: (a) dilution, (b) advection
Chemical Processes	(1) Processes represented: (a) coupled BOD-DO reactions; (2) Constituents represented: (a) carbonaceous BOD, (b) dissolved oxygen, (c) nitrogenous BOD
Ecological Processes	(1) Processes represented: (a) only first order biological decay represented, (b) effects of photosynthesis and benthic demand on DO levels not represented
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) LaGrangian evaluation of analytically integrated equations and mass balance
Computation Status	(1) Model coded in FORTRAN IV (G level); (2) Equipment requirements: (a) digital computer with 27,000 word storage capacity, (b) FORTRAN IV compiler, (c) no tapes or disks
Input Data Requirements	(1) Initial setup/calibration: (a) reach length, (b) mean velocity, (c) mean discharge, (d) mean depth per reach, (e) average reach temperature, (f) residuals discharge inflows, (g) withdrawals and distributed inflows, (h) residuals inputs as BOD, (i) dissolved oxygen concentration in each reach; (2) Verification: (a) streamflows, (b) stream velocity, (c) observed constituent concentrations throughout the modeled area
Ease of Application	(1) Model documentation: (a) documentation report available without charge from Texas Development Board, Austin, Texas, or EPA, Washington, D.C.; (2) Documentation contents: (a) theory, (b) subroutines, (c) file and data deck design, (d) program listings; (3) Modifications: (a) little recomputation time needed for data deck changes, (b) model very difficult to modify for additional constituents, both mathematically and in coding
Output and Output Format	(1) Output information: (a) concentration of dissolved oxygen in each reach, (b) carbonaceous and nitrogenous BOD at start and end of each reach; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Model cannot handle nonpoint residuals discharges except as tributary inputs (incremental runoff inputs)
Manpower Needs	(1) Requires one junior-level engineer with some basic programming experience
Costs	(1) Model acquisition: (a) reports may be free or nominal charge (0-$5); (2) Model setup and data preparation: (a) 2-6 man-weeks; (3) Actual computation: $1-5 per run; (4) Output analysis: (a) small, e.g., less than one man-hour
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes first order decay only; (2) Sensitivity: (a) high estimated sensitivity to residuals loads, velocities, (b) moderate estimated sensitivity to flow and decay coefficients
Other Comments	(1) DOSAG-I developed by Water Resources Engineers, Austin, Texas and Texas Water Development Board, Austin; (2) DOSAG has flow augmentation option to determine dilution flows needed to reach DO standard

Table 4-4. Summary of the Revised Dissolved Oxygen Sag Model (DOSAG-3)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Water conveyance canals
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal variation only; (3) Morphology: (a) DOSAG-3 permits no stratification (each reach well-mixed), (b) branched watershed network can be simulated
Time Properties	(1) Time variability: (a) steady state; (2) Time units of application: (a) variable depending upon total length of the system and prescribed flow
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) up to 49 stretches, (b) maximum of 80 reaches, (c) maximum of 20 headwaters, (d) up to 20 reaches per stretch
Physical Processes	(1) Principal driving force: (a) net downstream flow; (2) Processes represented: (a) advection, (b) dilution
Chemical Processes	(1) Processes represented: (a) chemical interactions, both coupled and uncoupled; (2) Constituents modeled: (a) dissolved oxygen, (b) carbonaceous BOD, (c) nitrogenous BOD, (d) phosphorus, (e) ammonia, (f) nitrite, (g) nitrate, (h) conservative materials--total N, chlorides, metal ions, e.g., iron
Ecological Processes	(1) Processes represented: (a) photosynthesis, represented by chlorophyll A, (b) coliform die-off, (c) first order bacterial decay, (d) algal respiration; (2) Trophic levels: (a) only decomposers and primary producers simulated; (3) Water quality-biota relationships represented: (a) algal (chlorophyll A)/nutrient dynamics
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) analytical integration (Laplace transforms), (b) utilizes LaGrangian approach where computations performed on reach by reach basis (progressing downstream)
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 27,000 word storage capacity, (b) FORTRAN IV compiler, (c) no disks or tapes
Input Data Requirements	(1) Initial setup/calibration: (a) reach length, (b) mean discharge, (c) mean reach velocity, (d) mean reach depth, (e) average reach temperature, (f) residuals discharge inflows, (g) withdrawals and groundwater inflows, (h) constituent concentrations in all inflows, (i) initial constituent concentrations by reach; (2) Verification: (a) observed streamflow, (b) observed stream velocities, (c) observed constituent concentrations throughout the modeled area
Ease of Application	(1) Model documentation: (a) documentation report available from EPA, Systems Development Branch, Washington, D.C.; (2) Documentation contents: (a) complete documentation contains theory, subroutine descriptions, file and data deck design, program listings, and sample problem; (3) Modifications: (a) little recomputation time needed for data deck changes
Output and Output Format	(1) Output information: (a) constituent concentrations in each reach, (b) flow rate, (c) reach depth, (d) minimum dissolved oxygen value and river mile where it occurs, (e) mean velocity, (f) algae growth rate; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Model cannot handle nonpoint residuals discharges except as tributary inputs (incremental runoff inputs)
Manpower Needs	(1) Requires one junior-level engineer with some basic programming experience
Costs	(1) Model acquisition: (a) documentation reports may be obtained for a nominal charge from EPA, Washington, D.C. or Water Resources Engineers, Austin, Texas; (2) Model setup and data preparation: (a) requires 2-7 man-weeks; (3) Actual computation: (a) $2-8 per simulation run; (4) Output analysis: (a) small, e.g., less than one hour
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes constant stream velocity throughout a reach, (b) assumes first order decay only; (2) Sensitivity: (a) high sensitivity to residuals inputs, stream velocities, (b) moderate sensitivity to flow and decay coefficients
Other Comments	(1) Limitations: (a) DOSAG-3 cannot compute nitrogenous BOD and other nitrogen species (ammonia, nitrite, nitrate) simultaneously; (2) Optional features: (a) flow augmentation option to reach prescribed DO standards, (b) model permits three different treatment efficiencies for residuals discharges; (3) DOSAG-3 derived from DOSAG-I by Water Resources Engineers, Austin, Texas

Table 4A-5. Summary of the SCI Modification of the Dissolved Oxygen Sag Model (DOSCI)

Characteristic	Summary Data
Applicable Water Body	(1) Rivers; (2) Streams
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal boundaries only; (3) Morphology: (a) no lakes or reservoirs can be modeled along the mainstem river, (b) no diffusion or stratification simulated because each reach is considered uniformly mixed
Time Properties	(1) Time variability: (a) steady state
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) 10 headwaters, (b) 20 junctions, (c) 20 stretches, (d) 100 reaches and inflows
Physical Processes	(1) Principal driving force: (a) net downstream flow; (2) Processes represented: (a) advection, (b) dilution, (c) settling, (d) reaeration
Chemical Processes	(1) Processes represented: (a) both coupled and uncoupled chemical reactions, (b) permits first and second order decay rates; (2) Constituents represented: (a) dissolved oxygen, (b) carbonaceous BOD, (c) ammonia, (d) nitrite, (e) nitrate, (f) orthophosphate, (g) three heavy metals--lead, copper, zinc, (h) five conservatives, including total nitrogen, chlorides; (3) Temperature-dependent reactions adjusted for each reach
Ecological Processes	(1) Processes represented: (a) first order bacterial decomposition, (b) photosynthesis, (c) coliform die-off, (d) benthic uptake and release; (2) Trophic levels: (a) only decomposer and primary producer dynamics permitted; (3) Water quality-biota relationships represented: (a) algal/nutrient and microbial uptake/regeneration interactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) combination of analytically integrated LaGrangian equations and mass balance equations, (b) computations for quantity and quality performed simultaneously on reach by reach basis, progressing downstream
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 27,000 word storage capacity, (b) FORTRAN IV (G level) compiler, (c) no tapes or disks, (d) previous applications run on UNIVAC 1108, IBM 370/155, and IBM 360/65 systems
Input Data Requirements	(1) Initial setup/calibration: (a) flow rates for all inflows and withdrawals, (b) constituent concentrations in all inflows and withdrawals, (c) stream temperature by reach, (d) groundwater or nonpoint inputs (treated as ten equally-spaced point source discharges along the reach), (e) decay and reaction rate coefficients, (f) cross-sectional area of stream, (g) lengths of each reach, (h) average solar radiation; (2) Verification: (a) simultaneous data on stream flow, velocity, depth, and constituent concentrations thoughout the modeled system
Ease of Application	(1) Model documentation: (a) documentation available in Vols. I and IV of Final Report on the Spokane River Basin Model Project to EPA Planning Assistance Branch, Washington, D.C., (2) Documentation contents: (a) does not provide program listings for Snohomish application; (3) Modifications: (a) all seventeen subroutines well-documented to facilitate changes, (b) decay and reaction rate terms may be calculated through equations provided in the documentation or user may utilize generalized values provided, (c) few card changes necessary or little recomputation time used to alter program
Output and Output Format	(1) Output information: (a) minimum DO level in reach and river mile where this depression occurs, (b) concentrations at start and end of reach for all quality constituents (concentration output is quality level just before the next downstream segment), then residuals inputs are added to form the basis for the inflow to the next reach, (c) reaction rate coefficient for reach, (d) travel time through reach, (e) slope of stream bottom, (f) all input values, (g) flow augmentation (quantity) to reach DO standard throughout system (optional), (h) user-specified plots of the various constituent concentrations vs. river mile; (2) Output format: (a) tabular printout, (b) plots
Linkages to Other Models	(1) DOSCI cannot handle dynamic residuals inputs or distinguish between or among spatial differences in residuals discharges
Manpower Needs	(1) Requires programmer or engineer with basic programming skills; (2) Experience in water quality data collection necessary if new field data being collected for calibration/verification
Costs	(1) Model acquisition: (a) nominal charge for documentation reports from EPA Planning Assistance Branch; (2) Model setup and data preparation: (a) may take only 3-5 man-days, (b) data gathering and preparation will require 3-7 man-weeks, depending on the size of the modeled system, data availability, and number of constituents being simulated; (3) Actual computation: (a) ranges between $2-10 per run (average run might involve 10-15 CPU seconds for $5); (4) Output analysis: (a) less than one man-hour per run if plotting subroutines utilized

Table 4A-5. DOSCI (continued)

Characteristic	Summary Data
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes constant stream velocity throughout the reach, (b) no vertical or lateral flow or quality variations, (c) assumes first order decay for BOD and non-nutrient constituents; (2) Sensitivity: (a) model sensitive to ammonia volatilization coefficient, residuals loads (estimated), flow velocities (estimated), (b) moderate sensitivity to streamflow, decay coefficients, reaeration coefficient (estimated)
Other Comments	(1) DOSCI is a variation of DOSAG used by Systems Control, Inc.; (2) SNOGCI is the acronym used to identify the DOSCI application to the Snohomish River Basin, Washington; (3) Like DOSAG, DOSCI has a flow augmentation option which calculates the amount of water inflow needed to maintain the dissolved oxygen level at a specified standard; (4) Later versions have optional temperature feature for assessing excess heat from power plants (DOSCI does allow different reach temperatures)

Table 4A-6. Summary of the Estuary Model (ES001)

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) Morphology: (a) handles riverine estuaries well, especially when net velocity is less than one foot per second
Time Properties	(1) Time variability: (a) steady-state
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) up to 100 junctions, (b) up to 100 segments (similar to reach), (c) maximum segment length of 20 miles
Physical Processes	(1) Principal driving force: (a) net flow; (2) Processes represented: (a) advection, (b) longitudinal dispersion, (c) dilution, (d) temperature effects
Chemical Processes	(1) Processes represented: (a) intercoupled DO/BOD reaction with first order kinetics, (b) BOD-DO levels affected by demands and releases of algal and benthic components; (2) Constituents represented: (a) DO, (b) BOD
Ecological Processes	(1) Processes represented: (a) algae effects on DO levels, (b) benthic effects on ambient DO or BOD concentrations
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) matrix inversion of simultaneous differential equations
Computation Status	(1) Model coded in Fortran IV; (2) Equipment requirements: (a) model prepared for use on IBM 370 series computer, (b) later versions of this model can be run on IBM 1130
Input Data Requirements	(1) Initial setup/calibration: (a) estuary cross-sectional area, (b) segment length, (c) water depth, (d) net flow, (e) reservoir outflows (f) estuary volume, (g) tidal exchange coefficient, (h) dispersion coefficient, (i) constituent concentrations for all system inflows, (j) temperatures, (k) benthic oxygen demand, (l) photosynthesis, respiration, and other rate coefficients, (m) residuals inputs from point sources, (n) uniform residuals inputs from nonpoint sources, (o) salinities at seaward boundaries, (p) temperature correction factors; (2) Verification: (a) constituent concentrations throughout the system, (b) observed salinity patterns
Ease of Application	(1) Model documentation: (a) documentation report available from EPA Region II, Systems Data Branch; (2) Documentation contents: (a) presents theoretical background, but associated verification report furnishes little assistance in new applications; (2) Modifications: (a) few card changes necessary, (b) short recomputation times for data deck changes, (c) documentation has limited comment statements, but adequate description of subroutines
Output and Output Format	(1) Output information: (a) BOD concentration and DO deficits at ten equidistant points per segment, (b) listings of input data without headings; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Model handles only steady-state residuals inputs from point and nonpoint sources; (2) Simple steady-state stream model might supply upstream inputs into this estuary model
Manpower Needs	(1) Requires computer programmer or engineer with basic programming skills
Costs	(1) Model acquisition: (a) documentation and verification reports available from EPA Region II, New York for nominal cost; (2) Model setup and data preparation: (a) 2-6 man-weeks required depending on the application; (3) Actual computation: (a) maximum of $10 for highly discretized system; (4) Output analysis: (a) probably less than one man-hour per simulation run
Model Accuracy and Sensitivity	(1) Representativeness: (a) handles only steady-state flows and discharges, (b) does not consider flow velocity or quality variations with depth or within stream cross-section, (c) assumes only first order kinetics for BOD and DO; (2) Sensitivity: (a) highly sensitive to reaeration coefficient, (b) also sensitive to the dispersion coefficient, net flow velocity, and deoxygenation coefficient
Other Comments	(1) ES001 has options to permit various kinds of sections and junctions that allow the user to examine the effects of completely mixed bays; (2) ES001 derived from previously-developed Hydroscience models

Model 4A-7. Summary of the River Quality Model (QUAL-I)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Converging water conveyance systems
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal boundaries only; (3) Flows: (a) only time invariant inflows and point source discharges considered; (4) Morphology: (a) mainstem stream may have several tributary branches, (b) each stream segment is considered well-mixed
Time Properties	(1) Time variability: (a) quasi-steady state--stream flows, inflows, withdrawals, discharges, and other hydrologic variables are time invariant, meteorological conditions can vary; (2) Time units of application: (a) meteorological inputs may be on an hourly basis or less frequent (3 hrs. common), (b) time step based on length = one travel time through the simulated system (3 hrs. common)
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (1) Discretization limits: (a) up to 25 reaches, (b) up to five junctions, (c) up to five headwaters, (d) up to 25 point discharges or withdrawals
Physical Processes	(1) Principal driving force: (a) net downstream flow (dispersion coefficient calculated internally from flow properties); (2) Processes represented: (a) advection, (b) dilution, (c) temperature effects (heat budget)
Chemical Processes	(1) Processes represented: (a) coupled BOD-DO reactions; (2) Constituents represented: (a) DO, (b) BOD, (c) three unspecified conservatives; (3) Temperature effects and reaeration important to chemical reactions
Ecological Processes	(1) Processes represented: (a) first order microbial decay for BOD; (2) Trophic levels: implied representation of decomposers
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference
Computation Status	(1) Model coded in Fortran IV (G level); (2) Equipment requirements: (a) digital computer with storage capacity of 35,000 words, (b) Fortran IV compiler
Input Data Requirements	(1) Initial setup/calibration: (a) headwater flows, (b) discharges inflows and withdrawals (c) stream depth, width and bottom roughness, (d) constituent concentrations and temperatures at headwaters, (e) residuals discharges with flows and concentrations constant, (f) BOD decay and other kinetic parameters, (g) weather conditions, (h) evaporation coefficients, (i) initial conditions, (j) treatment factors; (2) Verification: (a) flows throughout the modeled area, (b) concentrations of water quality constituents throughout the modeled area
Ease of Application	(1) Model documentation: (a) documentation report available from Texas Water Development Board (TWDB), Austin, Texas or EPA Planning Assistance Branch, Washington, D.C.; (2) Documentation contents: (a) good theory, data deck design, and helpful subroutines present in reports; (3) Modifications: (a) card changes necessary only for weather conditions or residuals loads, (b) recomputation time short for data deck changes
Output and Output Format	(1) Output information: (a) concentrations of constituents and temperatures in each reach at specified time steps, (b) final concentrations and temperatures at the end of simulation, (c) average kinetic parameters per reach used in each simulation; (2) Output format: (a) tabular printout, (b) optional plot package on TWDB version
Linkages to Other Models	(1) QUAL I may be upgraded into more complex ecologic-water quality model (see QUAL II) by adding extra constituents; (2) Model handles only constant residuals discharges or nonpoint source additions (as distributed inflows)
Manpower Needs	(1) Requires one computer programmer and/or environmental engineer with basic programming expertise; (2) Previous experience in water quality models based on Fortran IV useful
Costs	(1) Model documentation: (a) documentation reports available free from Texas Water Development Board, nominal charge for photocopying if originals no longer available; (2) Model setup and data preparation: (a) 2-5 man-weeks depending upon the extent of available quality data; (3) Actual computation: (a) $5-$50 per simulation run, depending upon system discretization and number of constituents modeled; (4) Output analysis: (a) small, usually less than one man-hour per simulation run
Model Accuracy and Sensitivity	(1) Representativeness: (a) handles only steady-state flows and discharges, (b) does not consider flow velocity or quality variations with depth or within stream cross-section; (2) Accuracy: (a) unconditionally stable, (b) low numerical dispersion; (3) Sensitivity: (a) estimated sensitivities--high for residuals loads and flow velocities, moderate for stream flow and decay coefficients, and low for depth, reaeration rate, and friction coefficient, (b) temperature simulation shows high sensitivity to depth and weather conditions
Other Comments	(1) QUAL I has flow augmentation option to determine flow rates needed to achieve specified DO levels; (2) Model developed by Texas Water Development Board, Austin, Texas

Model 4A-8. Summary of the Dynamic Estuary Model (DEM)

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries; (2) Rivers; (3) Nonsteep streams
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) does not possess capability to simulate tidal flats, (b) excellent for channelized situations; (3) Flows: (a) residuals inputs must be constant, (b) handles single recurring tidal cycle
Time Properties	(1) Time variability: (a) dynamic, (b) can be used for constant inflows-withdrawals; (2) Time units of application: (a) timesteps used in days, (b) hydrodynamics computed for single tide cycles
Space Properties	(1) Dimensionality: (a) pseudo two dimensions with one-dimensional channels, horizontal plane; (2) Discretization limits: (a) link-node network permits up to 1300 channels and 840 junctions for hydrodynamic module, (b) water quality module limited to 200 junctions and 400 channels
Physical Processes	(1) Principal driving forces: (a) net flow, (b) tidal movements; (2) Processes represented: (a) dilution, (b) advection, (c) diffusion
Chemical Processes	(1) Processes represented: (a) coupled and uncoupled reactions; (2) Constituents represented: (a) DO, (b) temperature, (c) BOD, (d) NH_2, (e) NO_3, (f) phosphate, (g) pesticides, (h) heavy metals, (i) chlorophyll a, (j) dissolved solids, (k) total nitrogen, (l) coliform bacteria (based on Pearl Harbor version), (m) user-specified water quality parameters (conservative or nonconservative with 1st order decay)
Ecological Processes	(1) Processes represented: (a) algal dynamics, (b) coliform die-off, (c) biological decay (1st order); (2) Trophic levels: (a) primary producers and decomposers are only trophic groups represented; (3) Water quality-biota relationships represented: (a) algal-nutrient interactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, explicit
Computation Status	(1) Model coded in Fortran IV; (2) Equipment requirements: (a) digital computer with 50,000 word storage, (b) Fortran IV compiler, (c) two tapes or disks
Input Data Requirements	(1) Initial setup/calibration: (a) headwater and tributary flows, (b) water withdrawals, (c) groundwater inflows, (d) seaward tides, (e) depths, (f) widths, (g) bottom roughness for each channel, (h) constituent concentrations at land boundary points (constant), (i) variable constituent concentrations at tidal boundaries, (j) residuals discharges flow and quality (constant), (k) first order decay rates for nonconservative constituents; (2) Verification: (a) net flows, (b) velocities, (c) constituent concentrations within the modeled area, (d) dye tracer study data for seaward boundary conditions
Ease of Application	(1) Model documentation: (a) documentation reports available from EPA Planning Assistance Branch or Water Resources Engineers, Austin, Texas or Walnut Creek, Calif., (2) Documentation contents: (a) complete description of theory, subroutines, data deck design, and program listings; (3) Modifications: (a) small recomputation time needed for card changes, (b) preparation of data deck requires considerable time
Output and Output Format	(1) Output information: (a) maximum and minimum flows, head, velocities, net flow, (b) maximum, minimum, and average constituent concentrations at each junction for each tidal cycle, (c) additional data at prescribed time intervals, such as channel flow; (2) Output format: (a) tabular printout, (b) channel velocities also transferred to tape
Linkages to Other Models	(1) DEM water quality module linked to Tidal Temperature Model for heat budget
Manpower Needs	(1) Requires one programmer and one environmental engineer with experience in water quality modeling
Costs	(1) Model acquisition: (a) nominal charge, e.g., $5-$20, for report if originals available; (2) Model setup and data preparation: (a) 5-20 man-weeks; (3) Actual computation: (a) depends upon needed system size and number of tidal cycles considered, (b) hydrologic--$20-$300/run, (c) quality--$10-$100/run; (4) Output analysis: (a) one man-week
Model Accuracy and Sensitivity	(1) Representativeness: (a) does not handle wind stress, tidal flats exposed at low tide, lateral and vertical variation within channels, (b) assumes instantaneous mixing of residuals discharges throughout section, (c) utilizes connected one-dimensional channels to simulate two-dimensional flow and transport; (2) Accuracy: (a) model conditionally stable, relationships between time step and channel depth critical, (b) numerical dispersion problems do occur; (3) Sensitivity: (a) model sensitive to quality time step size, net flow, residuals loading rates, (b) low sensitivity to quantity time step size, diffusion coefficients, friction coefficient, initial conditions
Other Comments	(1) DEM comprised of two distinct but compatible programs--hydraulics (DYNHYD) and quality (DYNQUAL); (2) Originally developed by Water Resources Engineers and modified for additional constituents for FWQA (EPA) for application to San Francisco Bay and Pearl Harbor

Table 4A-9. Summary of the Tidal Temperature Model (TTM)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Well-mixed shallow impoundments; (3) Estuaries; (4) Coastal waters
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) handles only non-steep streams, (b) cannot handle tidal flats that go dry; (3) Flows: (a) all inflows or withdrawals must be constant, (b) handles a single recurring tidal cycle, (c) handles only constant residuals input rates
Time Properties	(1) Time variability: (a) dynamic, except for constant residuals input rates
Space Properties	(1) Dimensionality: (a) pseudo two dimensions, horizontal plane; (2) Discretization limits: (a) up to 300 channels, (b) up to 300 junctions
Physical Processes	(1) Principal driving forces: (a) tides, (b) net river flow; (2) Processes represented: (a) advection, (b) diffusion, (c) dilution, (d) heat budget, (e) meteorological conditions
Chemical Processes	(1) Processes represented: (a) coupled BOD-DO reactions; (2) Constituents represented: (a) four unspecified constituents--each may be conservative or nonconservative, have coupled or noncoupled reactions, and undergo first order decay (nonconservative)
Ecological Processes	(1) None
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: finite difference, explicit
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 50,000 word storage capacity, (b) FORTRAN IV compiler
Input Data	(1) Initial setup/calibration: (a) headwater flows, (b) tributary flows, (c) groundwater flows, (d) water withdrawals, (e) seaward tides, (f) channel depths and widths, (g) bottom roughness, (h) constituents in freshwater inflows and at seaward boundaries, (i) constituents concentrations throughout the modeled area, (j) residuals discharges (point-source)--quality and quantity, (k) weather--net solar radiation, wet and dry bulb temperatures; (2) Verification (data taken at points throughout the modeled area): (a) net flows, (b) velocities, (c) ambient constituent concentrations, (d) dye studies of seaward boundary input conditions, (e) observed salinity regimes
Ease of Application	(1) Model documentation: (a) reports available from EPA Environmental Research Lab., Corvallis, Oregon; (2) Documentation contents: (a) good discussion on theory and application of the model, (b) model program is long and detailed, but some helpful comment statements and subroutines are available, (c) preparation of the input deck not clearly explained; (3) Modifications: (a) few card changes needed except for meteorological conditions, (b) little recomputation time necessary for card changes
Output and Output Format	(1) Output information: (a) summarized data--maximum and minimum values--for tidal cycle, flows, velocities, water elevation, (b) constituent concentrations at each junction, (c) flows, channel velocities, junction depths, and constituent concentrations at user specified time periods; (2) Output format: (a) tabular printout, (b) velocities written on tape by the hydrodynamic module
Linkages to Other Models	(1) Model primarily links hydrodynamic and temperature/heat budget components, but additional water quality constituents may be possible (see DEM)
Manpower Needs	(1) Requires one experienced programmer and one engineer experienced in hydrodynamics and water quality modeling
Costs	(1) Model acquisition: (a) nominal charge for program documentation reports from EPA; (2) Model setup and data preparation: (a) requires 5-20 man-weeks of effort, depending on familiarity with TTM, data availability, and size of the modeled system; (3) Actual computation: (a) $20-$300 per run for hydrodynamics (costs slightly more than DEM runs, but cost is dependent upon the number of channels and junctions); (4) Output analysis: (a) several man-hours needed for each output evaluation
Model Accuracy and Sensitivity	(1) Representativeness: (a) neglects wind stress, (b) disregards lateral and vertical variation in channel cross-sectional area with tidal elevation change, (c) assumes simplified evaporation, (d) assumes interconnected one-dimensional channels to represent two-dimensional flow and transport; (2) Accuracy: (a) conditionally stable but time intervals must be less than L/gh, (b) moderate to high numerical dispersion; (3) Sensitivity: (a) sensitive to quality time step size, (b) high estimated sensitivity to net flows and residuals discharge levels, (c) moderate estimated sensitivity to tides and headwater concentrations, (d) insensitive to friction coefficient, channel lengths, and initial conditions
Other Comments	(1) TTM is a derivative of the Dynamic Estuary Model that can simulate the heat budget; (2) Model developed by EPA Pacific Northwest Laboratory and has been applied to the Columbia River below Bonneville Dam; (3) TTM consists of two distinct but linked programs--HYDRA (basic hydrodynamics) and QUALTEMP (water quality including temperature); (4) Although temperature varies within the modeled aquatic system, temperature-dependent reaction rates do not change

Table 4A-10. Summary of the Receiving Water Model Module of SWMM (RECEIV)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Estuaries; (4) Marshes/swamps; (5) Lakes
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal boundaries, (b) can simulate estuarine flats at low tide by varying cross-sectional area; (3) Flows: (a) handles unsteady inflows such as residuals discharges, storm runoff, tides; (4) Morphology: (a) does not consider stratified systems, (b) considers ocean tide exchange at up to 20 input points
Time Properties	(1) Time variability: (a) dynamic, (b) option available for steady state conditions; (2) Time units of application: (a) 50 time-variable inputs possible exclusive of tidal variations
Space Properties	(1) Dimensionality: (a) pseudo two dimensions with interlocking one-dimensional channels, horizontal plane; (2) Discretization limits: (a) up to 225 channels, (b) up to 100 junctions in link-node network
Physical Processes	(1) Principal driving forces: (a) net flow, (b) tides,as a single recurring tidal cycle; (2) Processes represented: (a) advection, (b) dilution, (c) reaeration by O'Connor-Dobbins equation, (d) flows, tidal movements, and water surface changes, (e) wind stress and direct rainfall inputs, (f) lacks ability to simulate temperature
Chemical Processes	(1) Processes represented: (a) coupled and uncoupled chemical interactions, (b) considers only first order decay of constituents; (2) Constituents represented: (a) DO, (b) BOD, (c) four unspecified conservative or nonconservative substances; (3) All constituent concentrations must be specified in mg/l units except coliforms
Ecological Processes	(1) No biochemical processes simulated except BOD decay
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, explicit
Computation Status	(1) Model coded in FORTRAN IV-G level; (2) Equipment requirements: (a) computer with 50,000 word core storage capacity, (b) FORTRAN IV-G level compiler, (c) two magnetic tapes or disks
Input Data Requirements	(1) Initial setup/calibration: (a) constant or variable headwater inflow rates, (b) flow rate for each inflow (discharge, tributary, etc.) or withdrawal, (c) tidal cycles and heights at the seaward boundaries, (d) width, Manning roughness, and depth of each channel, (e) initial flow velocities and water surface elevations throughout the system, (f) initial constituent concentrations throughout the system, (g) residuals loading rates from discharges, tributaries, and headwaters, (h) tidal exchange coefficient, (i) meteorological data--wind direction and speed, rainfall, (k) first order decay rates for constituents; (2) Verification: (a) stage, net flow, and velocities, (b) constituent concentrations throughout the modeled system, (c) salinity data to establish concentration inputs at seaward boundary
Ease of Application	(1) Model documentation: (a) Storm Water Management Model (SWMM) documentation reports can be obtained from EPA Environmental Research Laboratory, Cincinnati, Ohio, or EPA Planning Assistance Branch, Washington, D.C., (b) original program description located in SWMM package; (2) Modifications: (a) inadequate documentation will make modifications difficult, (b) few card changes necessary except for time-varying residuals inputs, (c) little recomputation time required following card changes, (d) quality and quantity modules may be run separately
Output and Output Format	(1) Output information: (a) time step, net flow and velocities for each tidal cycle, (b) water surface elevation for selected junctions for each tidal cycle, (c) maximum, minimum, and average constituent concentrations at each junction per tidal cycle, (d) computed reaeration coefficients and DO saturation values; (2) Output format: (a) tabular printout, (b) line printer plots of junction stages and concentrations, (c) hydrodynamic output (esp. channel flows) may be written on magnetic tape or disk
Linkage to Other Models	(1) RECEIV is linked to the terrestrial flow routing module of the Storm Water Management Model; (2) RECEIV can be utilized by itself to simulate dynamic conditions
Manpower Needs	(1) Requires one computer programmer and one hydraulic engineer with basic programming background; (2) Previous experience with FORTRAN water quality models useful
Costs	(1) Model acquisition: (a) nominal charge ($10) for SWMM documentation report from EPA; (2) Model setup and data preparation: (a) 1 to 5 man-months needed depending on system complexity; (3) Actual computation: (a) hydrodynamic module costs between $15-$100 per run, (b) quality run ranges between $10-$50 per simulation run, (c) actual expense dependent upon extent of discretization, time step size, and length of simulation; (4) Output analysis: (a) several man-hours necessary to analyze output of each run
Model Accuracy and Sensitivity	(1) Representativeness: (a) can account for both steady state and dynamic conditions, (b) neglects lateral and vertical velocity variations within the channels, (c) assumes instantaneous mixing throughout each junction, (d) uses one-dimension channel network to simulate two-dimension flow and transport; (2) Accuracy: (a) low numerical dispersion noted, (b) conditionally stable if proper time step and channel geometry relationship used; (3) Sensitivity: (a) sensitive to quality time step size and decay coefficients, (b) estimated to be sensitive to residuals loading rates, headwater concentrations, net flow,and tides
Other Comments	(1) RECEIV is the receiving water module of the Storm Water Management Model (SWMM) developed by Water Resources Engineers, Metcalf and Eddy, and the University of Florida; (2) Special features: (a) model can handle transient stormwater loadings, (b) model can simulate tidal flats that go dry as well as marshes and swamps; (3) Model is currently maintained as part of the SWMM program by University of Florida, Gainesville

Table 4A-11. Summary of Systems Control, Inc. Modification of the Receiving Water Model (RIVSCI)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) does not consider stratified systems, (b) can simulate mud flats exposed at low tide and wind effects; (3) Flows: (a) can handle unsteady inflows e.g., residuals discharges, runoff, tides
Time Properties	(1) Time variability: (a) dynamic, (b) can also be used to simulate steady state conditions; (2) Time units of application: (a) only 20 time-variable inputs possible, exclusive of tide
Space Properties	(1) Dimensionality: (a) pseudo two-dimensions, horizontal plane; (2) Discretization limits: (a) 225 channels, (b) 100 junctions in the link-node system
Physical Processes	(1) Principal driving forces: (a) net downstream flow, (b) tides, as a single recurring tidal cycle; (a) Processes represented: (a) advection, (b) diffusion, (c) dilution
Chemical Processes	(1) Processes represented: (a) coupled reactions and first or second order decay/reaction kinetics, (b) temperature effects; (2) Constituents represented: (a) five conservative constituents, including total nitrogen and chlorides, (b) eleven nonconservative constituents--DO, BOD, ammonia, nitrite, nitrate, phosphate, fecal and total coliforms, copper, lead, zinc; (3) Decay and reaction rates may be user-specified (based on equations supplied in documentation)
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) growth, (c) biological decay--first or second order; (2) Water quality-biota relationships represented: (a) algal-nutrient dynamics
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, explicit numerical integration
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) computer with 50,000 word core storage, (b) two tapes or disks, (c) FORTRAN IV compiler, (d) previous applications have been run on UNIVAC 1108, IBM 370/155, and IBM 360/65
Input Data Requirements	(1) Initial setup/calibration: (a) flow rate for each inflow or withdrawal, (b) time history of the tide heights at the seaward boundary, (c) initial water surface elevations and velocities throughout the modeled system, (d) widths and initial depths of all channels, (e) evaporation rate and average wind speed (optional inputs), (f) concentrations of quality constituents in all inflows, (g) initial constituent concentrations, (h) decay and reaction rates, (i) water temperature at each junction, (j) tidal concentrations of the incoming tides as percentage of the previous outgoing tide (optional), (k) total daily solar radiation; (2) Verification: (a) concentrations of selected quality constituents throughout the modeled area taken simultaneously
Ease of Application	(1) Model documentation: (a) documentation reports available from EPA Planning Assistance Branch (Washington, D.C.), Snohomish County Planning Dept. (Washington), Systems Control, Inc. (Ca.); (2) Documentation contents: (a) original documentation (final report on Spokane River Basin Project) insufficient to describe model program; (3) Modifications: (a) hydrodynamic changes difficult, because majority of calculations in one large subroutine, (b) quality module has good documentation of all 18 subroutines
Output and Output Format	(1) Output information: (a) all initial inputs of hydrodynamic and quality parameters, (b) time history of channel flows, velocities, and junction volumes, (c) plots of surface elevation of junctions vs. time, (d) concentrations of constituents at each junction at specified time steps (daily maximum, minimum, and average concentrations); (2) Output format: (a) tabular printout, (b) plots, (c) SWFLOW hydrodynamics written on tape or disk for input into SWQUAL computation; (3) User may specify the frequency of output and the number of junctions and channels for which information will be presented
Linkages to Other Models	(1) RIVSCI can be linked to the terrestrial flow routing component of the Storm Water Management Model
Manpower Needs	(1) Requires computer programmer or hydrologist with experience in water quality and with basic programming skills; (2) Field collection of data, especially for verification requires specialized training
Costs	(1) Model acquisition: (a) nominal charge for documentation reports from EPA or SCI; (2) Model setup and data preparation: (a) 5 to 20 man-weeks, depending upon system complexity and data availability, (b) verification data likely to require expensive field monitoring effort; (3) Actual computation: (a) variable--hydrodynamics ($15-100) and quality ($10-50), (b) depends on the extent of discretization, time step size, length of simulation, (c) sample cost--30 channel, non-estuarine system (one hour time step, 8-day simulation) required 30 CPU seconds on an IBM 370/155 for a cost of $10; (4) Output analysis: (a) unknown
Model Accuracy and Sensitivity	(1) Representativeness: (a) can simulate both steady state and dynamic conditions; (2) Accuracy: (a) conditionally stable if $\Delta t < L/gh$, (b) low numerical dispersion; (3) Sensitivity: (a) sensitive to input tide heights, large tributary flows, depths, slopes, Manning's coefficients, integration time step size, ammonia volatilization coefficient, BOD decay coefficient (somewhat), (b) high estimated sensitivity to net flow and residuals loading rates, (c) moderate sensitivity to tide and headwater concentrations of water quality parameters, (d) becomes less sensitive to reaeration coefficient as DO approaches saturation
Other Comments	(1) Model divided into two models: (a) SWFLOW--hydrodynamics, (b) SWQUAL--water quality; (2) RIVSCI has been verified only for non-estuarine steady state cases

Table 4 A-12. Summary of Water Resources Engineers Modification of the Receiving Water Model (WRECEV)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) longitudinal boundaries, (b) can simulate tidal flats by varying cross-sectional area; (3) Flow: (a) can handle both steady and unsteady flow, (b) possible to simulate runoff and time-varying residuals discharges, (c) only constant water withdrawals permitted, (4) Morphology: (a) cannot simulate vertical stratification, (b) considers ocean tide exchange at single input point
Time Properties	(1) Time variability: (a) dynamic, (b) steady state conditions also possible; (2) Time units of application: (a) hourly time steps common, (b) only 20 time-variable inputs possible
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) up to 225 channels, (b) up to 100 junctions in link-node network
Physical Processes	(1) Principal driving forces: (a) net downstream flow, (b) tides as a single recurring tidal cycle; (2) Processes represented: (a) advection, (b) dilution, (c) diffusion; (3) System hydrodynamics: (a) simulates flows, tidal movements, and water surface changes, (b) lacks ability to represent temperature/heat budget, (c) lacks wind stress, evaporation, and Coriolis acceleration factors
Chemical Processes	(1) Processes represented: (a) handles noncoupled chemical interactions, except for coupled DO-BOD reactions, (b) constituent reactions are confined to first order decay; (2) Constituents represented: (a) DO, (b) biological oxygen demand, (c) four additional user-specified constituents
Ecological Processes	(1) Processes represented: (a) coliform die-off (optional)
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, explicit
Computation Status	(1) Model coded in FORTRAN IV-G level; (2) Equipment requirements: (a) digital computer with 50,000 word storage capacity, (b) FORTRAN IV-G level compiler, (c) two magnetic tapes or disks
Input Data Requirements	(1) Initial setup/calibration: (a) constant headwater inflow rates, (b) flow rate for each inflow or withdrawal, (c) widths and depths of each channel, (d) initial water surface elevations (at nodes) and channel flow velocities, (e) tidal cycles and heights at the seaward boundary (if applicable), (f) initial consituent concentrations throughout the system, (g) residuals loading rates from discharges, tributaries, (h) tidal exchange coefficient (if applicable), (i) meteorological data--wind speed, rainfall, and solar radiation, (j) first order decay rates for constituents; (2) Verification: (a) net flow and velocities for each channel, (b) constituent concentrations throughout the modeled area, preferably taken at points corresponding to model nodes, (c) salinity data or dye tracer studies to establish constituent concentration inputs at seaward boundary (if applicable)
Ease of Application	(1) Model documentation: (a) complete documentation report available from EPA Planning Assistance Branch, Washington, D.C. or Water Resources Engineers, Austin, Texas; (2) Documentation contents: (a) theoretical model discussion, (b) subroutine descriptions, (c) data deck design, (d) sample problem, (e) program listings, (f) discussions of revisions to RECEIV; (3) Modifications: (a) complete documentation package helpful in using model alone or connected to other SWMM modules, (b) few card changes necessary except for time-varying flow and weather, (c) short recomputation time needed after card changes
Output and Output Format	(1) Output information: (a) maximum, minimum, and net flows for each tidal cycle (if applicable), (b) velocities and water surface elevations for each tidal cycle (if applicable), (c) flow, velocities and constituent concentrations in each channel at specified time intervals, (d) depth at each junction at specified time intervals; (2) Output format: (a) tabular printout, (b) certain output may be written on magnetic tape
Linkages to Other Models	(1) WRECEV receives inputs from the transport module and storage module of the Storm Water Management Model; (2) WRECEV can be run independently for simulation of unsteady flow conditions
Manpower Needs	(1) Requires one computer programmer and one experienced hydraulic water quality engineer, (2) Previous experience with FORTRAN water quality models useful
Costs	(1) Model acquisition: (a) approximately $25 for WRECEV documentation report from Water Resources Engineers or EPA; (2) Model setup and data preparation: (a) 1 to 5 man-months depending on model complexity; (3) Actual computation: (a) hydrodynamic application costs $15-100 per run, (b) quality runs cost $10-50 per simulation run, in addition to the cost of the hydrodynamic application; (4) Output analysis: (a) 1 to 3 man-hours necessary to analyze output
Model Accuracy and Sensitivity	(1) Representativeness: (a) uses one-dimensional channel network to represent two-dimensional flow and transport, (b) assumes instantaneous mixing throughout each junction, (c) neglects lateral and vertical velocity within channels, (d) can simulate both steady and nonsteady flow regimes; (2) Accuracy: (a) low numerical dispersion, (b) conditionally stable if proper relationship between time steps and system geometry established; (3) Sensitivity: (a) sensitive to quality time step size and decay coefficient, (b) sensitive to residuals loading rates, headwater concentrations, net flow and tides
Other Comments	(1) Special features: (a) WRECEV can handle transient stormwater loadings, (b) can simulate tidal flats that go dry (must remain dry for the entire time step); (2) Originators: (a) WRECEV is a modification of the Receiving Water Block of the Storm Water Management Model developed by Water Resources Engineers, Austin, Texas

Table 4A-13. Summary of the Deep Reservoir Model (DRM)

Characteristic	Summary Data
Applicable Water Body	(1) Lakes; (2) Man-made reservoirs
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) handles vertical variations in deep, multi-layer lake systems; (3) Morphology: (a) considers stratification, (b) can handle one, two, or three reservoir outlets, but only one tributary inflow (or none at all)
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) time steps must be in hours because longer periods lead to some model stability problems
Space Properties	(1) Dimensionality: (a) one dimension, vertical axis model; (2) Discretization limits: (a) 200 layers, (b) 365 days
Physical Processes	(1) Processes represented: (a) advection, (b) diffusion, (c) heat budget; (2) System hydrodynamics: (a) simulates hydrodynamics and temperature variations only
Chemical Processes	(1) None
Ecological Processes	(1) None
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 35,000 word storage capacity, (b) FORTRAN IV compiler
Input Data Requirements	(1) Initial setup/calibration: (a) reservoir length, (b) lake depth/area relationship, (c) outlet elevations, (d) historical water surface elevation (initial and maximum), (e) lake inflow rates and inflow temperatures (daily), (f) lake outlow rates, (g) initial temperature conditions, (h) extinction depth, (i) diffusion parameters, (j) weather--dewpoint, air temperature, evaporation coefficient, wind speed, atmospheric pressure, solar radiation; (2) Verification: (a) time-varying temperature profiles and ouflow temperatures
Ease of Application	(1) Model documentation: (a) reports available from EPA Planning Assistance Branch, Washington, D.C.; (2) Documentation contents: (a) three distinct volumes--user's manual, theoretical description, and user's manual for application to Dworshak Reservoir, (b) reports include useful comment statements, subroutines, etc.; (3) Modifications: (a) few card changes needed, principally weather changes, (b) little recomputation time involved for card changes
Output and Output Format	(1) Output information: (a) meteorology--net short-wave and long-wave radiation rates, net heat loss, evaporation rates, atmospheric vapor pressure, (b) hydrology--lake inflows, lake outflows, water surface and thermocline elevations, diffusion coefficient, (c) temperature--air and water surface temperatures, outlet and downstream temperatures, variations in temperature with depth; (2) Output format: (a) tabular printout, (b) magnetic tape
Linkages to Other Models	(1) DRM is predominantly hydrodynamic--temperature model which can be linked to water quality modules to produce a lake ecologic model
Manpower Needs	(1) Requires one computer programmer and one experienced hydraulic-water quality engineer
Costs	(1) Model acquisition: (a) nominal, e.g., less than $30 for reports; (2) Model setup and data preparation: (a) can be substantial, normally 8 to 15 man-weeks required; (3) Actual computation: (a) estimated at $30-100 per run; (4) Output analysis: (a) several man-hours required to evaluate each output
Model Accuracy and Sensitivity	(1) Representativeness: (a) neglects horizontal water movement and temperature profiles (2) Accuracy: (a) conditionally stable, but time steps less than one day in length are required, (b) low to moderate numerical dispersion; (3) Sensitivity: (a) moderate for the eddy conductivity coefficient
Other Comments	(1) Repetitive simulations possible if meteorological conditions are unchanged; (2) Model originally developed by WRE for California Dept. of Fish and Game and refined in later work for EPA and the U.S. Army Corps of Engineers

Table 4A-14. Summary of the Lake Ecologic Model (LAKSCI)

Characteristic	Summary Data
Applicable Water Body	(1) Lakes; (2) Reservoirs
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) simulates multi-layered, stratified water bodies, (b) considers vertical variations between layers
Time Properties	(1) Time variability: (a) dynamic
Space Properties	(1) Dimensionality: (a) one dimension, vertical plane, (b) considers vertical variations only (2) Discretization limits: (a) maximum of 100 layers, (b) simulation period up to 365 days
Physical Processes	(1) Processes represented: (a) advection, (b) diffusion, (c) heat budget
Chemical Processes	(1) Processes represented: (a) coupled interactions between many quality constituents; (2) Constituents modeled: (a) nonconservatives--carbonaceous BOD, three unspecified heavy metals (first or second order decay), (b) conservatives--total N, chlorides, heavy metals
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) coliform die-off; (2) Water quality-biota relationships represented: (a) algal-nutrient relationships
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) combination of analytical and finite difference methods
Computation Status	(1) Model coded in FORTRAN IV-G; (2) Equipment requirements: (a) digital computer with 50,000 word storage capacity, (b) FORTRAN IV-G compiler
Input Data Requirements	(1) Initial setup/calibration: (a) lake inflow/outflow rates, (b) lake depth/area relationship, (c) lake length, (d) reservoir dam width and outlet heights, (e) water surface evaluations (initial and maximum), (f) daily inflow temperatures, (g) initial temperature conditions, (h) evaporation coefficients, (i) diffusion coefficients, (j) extinction depth, (k) initial constituent concentrations, (l) daily inflow constituent concentrations, (m) reaeration coefficients, (n) decay and settling rate coefficients, (o) temperature correction factors, (p) simulation dates, (q) reservoir elevation, latitude, and longitude, and (r) selected meteorology (dry and wet bulb air temperatures, short-wave solar radiation, atmospheric pressure, wind speed, sky cover); (2) Verification: (a) historical water surface elevations, (b) constituent concentrations in vertical lake profile and at lake outlets for several locations and time periods
Ease of Application	(1) Model documentation: (a) user's manual available from EPA Region X, Seattle, or Systems Control, Inc., Palo Alto, Ca.; (2) Documentation contents: (a) good theoretical discussion, user documentation, and model application results, (b) contains useful comment statements and subroutine descriptions; (3) Modifications: (a) recomputation time small for card changes, (b) option available for repeat simulations when meteorological conditions are unchanged
Output and Output Format	(1) Output information: (a) simulation date, (b) meteorological conditions, (c) water surface elevations, (d) lake inflows and outflows, (e) outflow temperatures, (f) outflow constituent concentrations, (g) constituent concentrations throughout the depth profile; (2) Output format: (a) tabular printout, (b) magnetic tape
Linkages to Other Models	(1) Lake outflows--quantity and quality--may serve as input into river models
Manpower Needs	(1) Requires computer programmer and/or water quality engineer; (2) Experience in water quality models based on FORTRAN IV helpful
Costs	(1) Model acquisition: (a) nominal charge for documentation reports from EPA Region X; (2) Model setup and data preparation: (a) may require substantial effort, e.g., 8 to 20 man-weeks; (3) Actual computation: (a) normal runs may range between $40 and $150 each (utilizing an IBM 370/55 during daytime hours); (4) Output analysis: (a) several man-hours required to evaluate each input
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes no horizontal flow velocities or horizontal quality variations, (b) assumes first order decay except for nutrients which may exhibit second order kinetics; (2) Accuracy: (a) conditionally stable if time steps are less than one day, (b) low numerical dispersion; (3) Sensitivity: (a) highly sensitive to time step size and BOD decay coefficient, (b) moderately sensitive to eddy conductivity coefficient, ammonia decay and volatilization coefficients, (c) low sensitivity to the reaeration coefficient
Other Comments	(1) LAKSCI is a modification of the Deep Reservoir Model developed for EPA by Systems Control, Inc., Palo Alto, Ca. for application to two lakes in the Spokane River Basin; (2) LAKSCI has the option for repetitive simulations if meteorological conditions are not changed

Table 4A-15. Summary of the Reservoir Water Quality Model (EPARES)

Characteristic	Summary Data
Applicable Water Body	(1) Lakes; (2) Reservoirs
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) handles vertical variations in deep, multi-layer lakes; (3) Morphology: (a) considers highly stratified systems
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) time steps must exceed one hour, (b) total simulation period limited to 365 days
Space Properties	(1) Dimensionality: (a) one dimension, vertical plane; (2) Discretization limits: (a) maximum of 10 lake inflows, (b) maximum of 10 lake outlets, (c) maximum of 100 layers
Physical Processes	(1) Processes represented: (a) advection, (b) diffusion, (c) heat budget
Chemical Processes	(1) Processes represented: (a) coupled and uncoupled chemical reactions; (2) Constituents represented: (a) three conservatives--chlorides, total N, unspecified metal ion, (b) non-conservatives--carbonaceous BOD, dissolved oxygen, ammonia, nitrite, nitrate, coliforms, phosphorus
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) algal respiration, (c) coliform die-off, (d) first order bacterial decay; (2) Trophic levels represented: (a) only decomposers and primary producers represented; (3) Water quality-biota relationships represented: (a) algal/nutrient interactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, implicit
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with 35,000 word storage capacity, (b) FORTRAN IV compiler, (c) magnetic tapes (if required)
Input Data Requirements	(1) Initial setup/calibration: (a) reservoir length, (b) lake depth/area relationship, (c) outlet elevations, (d) historical water surface elevation (initial and maximum), (e) lake inflow rates, (f) constituent concentrations and temperatures in lake inflows, (g) lake outflow rates, (h) constituent concentrations and temperatures in lake outflows, (i) initial lake conditions, (j) light extinction depth, (k) diffusion parameters, (l) meteorological conditions--air temperature, evaporation coefficient, wind speed, solar radiation; (2) Verification: (a) time-varying profiles of temperature and constituent concentrations throughout the lake, (b) temperatures and constituent concentrations at lake outputs
Ease of Application:	(1) Model documentation: (a) documentation report available from EPA Systems Development Branch, Washington, D.C. or WRE, Austin, Texas; (2) Documentation contents: (a) contains sketchy theoretical discussions and sample problem, (b) good presentation of program listings, data deck design, and associated MFIP data preparation program, (c) report should be supplemented with model documentation reports for DOSAG 3 (constituents) and Deep Reservoir Model (hydrodynamics-temperature); (3) Modifications: (a) few card changes needed except for weather, (b) little recomputation time required to implement card changes
Output and Output Format	(1) Output information: (a) initial conditions, (b) general system information--water surface elevation, total inflows and outflows, (c) meteorological data--solar radiation, air temperature, atmospheric pressure, wind speed, evaporation rate, (d) flow, temperature, and constituent concentrations of lake outflows, (e) algal growth and respiration rates, (f) diffusion coefficient; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Lake outflows may serve as input to downstream river model; (2) Lake inflows may be connected to upstream river model
Manpower Needs	(1) Requires one computer programmer experienced in FORTRAN and one experienced hydraulic water quality engineer
Costs	(1) Model acquisition: (a) nominal cost, e.g., less than \$20, for documentation report; (2) Model setup and data preparation: (a) can be substantial, e.g., 8 to 16 man-weeks; (3) Actual computation: (a) \$30-120 per run; (4) Output analysis: (a) several man-hours required to evaluate each output
Model Accuracy and Sensitivity	(1) Representativeness: (a) model neglects horizontal water movement and temperature-quality constituent variation, (b) system hydrodynamics directly related to temperature-water density relationships; (2) Accuracy: (a) model conditionally stable, but time steps of less than one day are necessary to ensure stability; (3) Sensitivity: (a) moderately sensitive to the eddy diffusion coefficient
Other Comments	(1) Model limitations: (a) temperature and water quality constituents must always be simulated together, (b) ammonia, nitrite, and nitrate must be simulated as a group; (2) Options: (a) repetitive simulations possible if meteorological conditions are unchanged; (3) EPARES is a derivative of the DRM, with the quality model from DOSAG 3; (4) EPARES developed by Water Resources Engineers, Austin, Texas for use on reservoirs in the Chattahoochee-Flint River Basin

Table 4A-16. Summary of Hydrocomp Hydrologic Simulation Program (HSP)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Lakes
Water Body Characteristics	(1) Scale: (a) far field; (2) Flows: (a) accounts for dynamic water movements, (b) overland water movement (runoff) simulated by LANDS program, (c) receiving waters simulated by CHANNELS program; (3) Morphology: (a) handles reservoir systems located along the mainstem river (limited to three layers), (b) each channel or reservoir layer considered well-mixed
Time Properties	(1) Time variability: (a) dynamic, including variable residuals and runoff inputs; (2) Time units of application: (a) hourly if runoff following rainfall event is being simulated
Space Properties	(1) Dimensionality: (a) one dimension, horizontal or vertical plane; (2) Discretization limits: (a) up to 150 channels, (b) 10 three-layer reservoirs, (c) 10 point source discharges, (d) diversions or withdrawals
Physical Processes	(1) Principal driving force: (a) net flow including runoff contributions; (2) Processes represented: (a) advection, (b) dilution, (c) heat budget, (d) precipitation, (e) groundwater flow, (f) interception, (g) evapotranspiration, (h) surface runoff, (i) evaporation
Chemical Processes	(1) Processes represented: (a) coupled interactions, (b) first and second order decay rates possible; (2) Constituents represented: (a) total dissolved solids, (b) dissolved oxygen, (c) BOD, (d) coliforms (three types), (e) ammonia, (f) nitrite, (g) nitrate, (h) orthophosphate, (i) potential phosphorus, (j) total nitrogen, (k) additional user-specified conservative substances
Ecological Processes	(1) Processes represented: (a) biological decay, (b) photosynthesis, (c) growth, (d) respiration, (e) mortality, (f) herbivore grazing; (2) Trophic levels represented: (a) decomposers, (b) primary producers, (c) herbivores (zooplankton)
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference numerical integration, except for overland flow based on Chezy-Manning equation
Computation Status	(1) Model coded in PL/1 language; (2) Equipment requirements: (a) IBM 360 or 370 computer system essential, (b) disk storage necessary (amount depends on size of input files), (c) hydrodynamics program (HSP) requires 64,000 word storage capacity, quality program requires additional 65,000 word storage capacity
Input Data Requirements	(1) Initial setup/calibration: (a) precipitation during simulation period, (b) flow rates for each inflow and withdrawal, (c) reservoir operating curve, (d) reservoir water surface elevation histories, (e) stream channel characteristics (cross-section, length, slope, Manning's roughness coefficient), (f) snowmelt factors such as water equivalent, snowpack depth, snow density, percentage snow cover, (g) evapotranspiration rates, (h) interception coefficients, (i) infiltration coefficients, (j) constituent concentrations in all inflows, (k) reaction and decay rate coefficients, (l) surface accumulation and washoff rate constants, (m) initial constituent concentrations and temperatures, (n) meteorological time history for temperature determination (solar radiation, maximum and minimum air temperatures, dewpoint temperatures, wind velocity, cloud cover); (2) Verification: (a) flow rates and constituent concentrations throughout the modeled area under both dry-weather and rainfall conditions
Ease of Application	(1) Model documentation: (a) report available from Hydrocomp International, Palo Alto, Ca., (b) model program proprietary and available on lease basis only; (2) Documentation contents: (a) quality documentation insufficient and necessitates consulting help for data disk preparation and verification; (3) Modifications: (a) changes to the basic program must be made by Hydrocomp according to the lease arrangement, (b) changes in input conditions in LIBRARY easy
Output and Output Format	(1) Output information: (a) time histories of flow, velocity, and channel depth (recorded on tape for LIBRARY), (b) time history of quality constituents, (c) reservoir data on surface elevation, overdam spill, controlled release, and inflow, (d) snow conditions (snow input data plus melt and liquid water, radiation exchange, rain or snow, condensation and convection melt, radiation melt, melt from rainfall, ground melt, and snow evaporation), (e) channel data on flow, travel time, depth, and velocity, (f) limiting nutrients for phytoplankton (light, phosphorus, or nitrogen); (2) Output format: (a) tabular printout, (b) plots available with appropriate subroutines, (c) LIBRARY stores hydrodynamic data on tape or disk for use in quality computations
Linkages to Other Models	(1) None
Manpower Needs	(1) Requires one experienced programmer and one competent water resources engineer; (2) Additional consulting support from Hydrocomp personnel needed for model setup, data preparation, and verification
Costs	(1) Model acquisition: (a) documentation report available for $15; however, model program is proprietary and available by annual lease only ($1250 + 20% of computer charges during model usage), (b) quality package to be used with HSP hydrodynamics available on annual lease for $600 + 15% of computer charges; (2) Model setup and data preparation: (a) considerable work effort needed to assemble necessary data (actual man-days unknown), (b) 30 hours of Hydrocomp technical assistance included in leasing arrangements; (3) Actual computation: (a) considerable due to large core storage requirements; (4) Output analysis: (a) unknown

Table 4A-16. HSP (continued)

Characteristic	Summary Data
Model Accuracy and Sensitivity	(1) Representativeness: (a) adequately represents streamflow conditions under both dry-weather flows and runoff due to precipitation within the watershed, (b) simulation of lakes greatly affected by mixing coefficients in the three-layered systems; (2) Sensitivity: (a) highly sensitive to meteorological conditions, (b) moderately sensitive to evapotranspiration, interception, and infiltration coefficients, (c) sensitivity to quality parameters currently unknown
Other Comments	(1) HSP is actually part of HSM, a three-program package consisting of HSP (hydrodynamics), QUALITY, and LIBRARY (data storage and retrieval system); (2) HSP was originally derived from the Stanford Watershed Model

Table 4A-17. Summary of the Coastal Circulation and Dispersion Model (CAFE/DISPER)

Characteristic	Summary Data
Applicable Water Body	(1) Wide rivers; (2) Lakes; (3) Nearshore coastal waters; (4) Estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) Morphology: (a) useful for simulating systems with completed topographical boundaries, (b) handles depth-averaged two-dimensional systems (one layer)
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) time steps computed in seconds, usually 100-second intervals
Space Properties	(1) Dimensionality: (a) two dimensions; (2) Discretization limits: (a) study area represented by finite element grid (triangular components) that can be assembled in any form (variable-sized grids possible), (b) maximum number of grids unknown (80 elements, 63 nodes used in examples)
Physical Processes	(1) Principal driving forces: (a) CAFE-I models circulation through a given area, i.e., (provides net volume flow through a given area, (b) DISPER-I traces path of discrete particles through the flow field; (2) Processes represented: (a) advection, (b) tidal movements, (c) wind-induced movements
Chemical Processes	(1) Processes represented: (a) both conservative and nonconservative substances can be traced through the flow field (user must specify appropriate dispersion and decay coefficients), (b) does not permit coupled water quality reactions
Ecological Processes	(1) No ecological processes possible, unless treated as discrete particles, e.g., fish larvae
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite element, numerical integration
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) computer requirements unspecified, probably IBM 360 or larger
Input Data Requirements	(1) Initial setup/calibration: (a) CAFE-I--mean low water depth at each node, bottom friction and eddy viscosity coefficients, tidal period, water density, latitude, tidal amplitude and phase lag, location and magnitude of water heights and flow, wind force over time, (b) DISPER-I--depth at each node, dispersion and decay coefficients, location, duration, and magnitude at boundary nodes, initial concentration at each node; (2) Verification: (a) unknown
Ease of Application	(1) Model documentation: (a) theory report and user's manual available from MIT Sea Grant Program Office, Cambridge, Mass.; (2) Documentation contents: (a) adequate theoretical description and mathematical formulations presented, (b) program files and data deck design present in user's manual
Output and Output Format	(1) Output information: (a) CAFE-I--current vectors at each node, (b) DISPER-I--particle paths through flow field; (2) Output format: (a) tabular printout, (b) cal-comp plots printed every 25 time steps
Linkages to Other Models	(1) CAFE-I links with water quality program through DISPER-I, but model best suited for hydrodynamic applications, (2) Model can simulate dynamic discharges of individual residuals
Manpower Needs	(1) Requires experienced programmer and hydraulic engineer with substantial experience in multi-dimensional flow; (2) High level of expertise in complex FORTRAN models desirable
Costs	(1) Model acquisition: (a) about $20 for documentation reports and user's manual; (2) Model setup and data preparation: (a) unknown, but manpower requirements may be large; (3) Actual computation: (a) unknown
Model Accuracy and Sensitivity	(1) Representativeness: (a) excellent systems representation by the variable finite element grid network; (2) Accuracy: (a) numerically stable if care is taken during discretization, grid setup and small time steps must be compatible
Other Comments	(1) Models developed at Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology, Cambridge, Mass. for NOAA, Office of Sea Grants Programs, Washington, D.C.; (2) Models considered operational only for hydrodynamics in REQM context, additional model building necessary for water quality analyses; (3) CAFE/DISPER model has been used for studies of particle entrainment through power plants

Table 4A-18. Summary of the Estuary Water Quality Model (EXPLORE-I)

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries; (2) Tidal rivers
Water Body Characteristics	(1) Scale: (a) far field; (2) Flows: (a) upstream river inflows may be time varying or steady; (3) Tides: (a) single tide function utilized, (b) permits tidal flats that dry up
Time Properties	(1) Time variability: (a) dynamic, (b) has option for steady state conditions; (2) Time units of application: (a) daily input values
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane (quasi two-dimensional in link-node network); (2) Discretization limits: (a) no limits specified
Physical Processes	(1) Principal driving forces: (a) net downstream flow, (b) tides; (2) Processes represented: (a) advection, (b) dilution, (c) wind stress
Chemical Processes	(1) Processes represented: (a) both coupled and noncoupled chemical reactions, (b) both first and second order decay of nutrients, (c) sedimentation and scour of organic matter (BOD); (2) Constituents represented: (a) DO, (b) BOD, (c) ammonia nitrogen, (d) nitrite nitrogen, (e) nitrate nitrogen, (f) total nitrogen, (g) salinity, (h) soluble phosphorus, (i) sulphite waste liquor, (j) toxic compounds
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) respiration, (c) biological decay, (d) coliform die-off; (2) Trophic levels: (a) only primary producers and coliform bacteria represented directly; (3) Water quality-biota relationships represented: (a) nutrient/chlorophyll a reactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, leap-frog explicit
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) IBM digital computer with unspecified core storage capacity
Input Data Requirements	(1) Initial setup/calibration: (a) net freshwater inflows, (b) tidal record at seaward boundary, (c) channel length and width, (d) mid-channel bottom elevation, (e) bottom roughness coefficient, (f) channel cross-section area, (g) initial flow velocities in system channel, (h) initial water surface elevations at each system junction, (i) initial constituent concentrations throughout the system, (j) meteorological data--wind speed and daily solar radiation, (k) seaward boundary coefficient for each constituent; (2) Verification: (a) net flow and velocities for each channel, (b) data records for stage heights for junction locations, (c) data record for constituent concentrations throughout the modeled system
Ease of Application	(1) Model documentation: (a) documentation reports can be obtained from Battelle Pacific Northwest Laboratories, Richland, or EPA, Planning Assistance Branch, Washington, D.C.; (2) Documentation contents: (a) four reports--System Layout and Data Report, Sensitivity Analysis Report, User's Manual, and Documentation Report for Grays Harbor Project, (b) program listings and source card decks also available from Battelle; (3) Modifications: (a) user's manual provides details for modifications, (b) few card changes needed unless time-varying inputs specified
Output and Output Format	(1) Output information: (a) water flow, flow velocities, and constituent concentrations for each channel at specified time intervals, (b) surface elevations at each junction at specified time intervals; (2) Output format: (a) tabular printout, (b) hydrodynamic output may be written on magnetic tape or disks
Linkages to Other Models	(1) EXPLORE-I application to Grays Harbor, Washington was linked to steady-state river model PIONEER-I to simulate the Chehalis River inflows
Manpower Needs	(1) Requires computer programmer or environmental engineer with some basic programming experience; (2) Water quality data collection program may require additional manpower
Costs	(1) Model acquisition: (a) cost of obtaining program and documentation reports from Battelle unknown; (2) Model setup and data preparation: (a) 2 to 8 man-weeks depending on data availability and constituent set modeled; (3) Actual computation: (a) unknown; (4) Output analysis: (a) only a few man-hours
Model Accuracy and Sensitivity	(1) Representativeness: (a) can simulate both steady state and dynamic conditions, (b) assumes diffusion to be negligible, (c) assumes mass transfers between nodes due solely to simple transport and water quality kinetics; (2) Accuracy: (a) stability is maintained if the appropriate time step maximum is not exceeded during link-node setup; (3) Sensitivity: (a) individual parameter sensitivities unknown (see Sensitivity Analysis Report)
Other Comments	(1) Special features: (a) user may select limited set of constituents including DO, SOD, salinity, coliforms, and toxic compounds, rather than the full set of 12 constituents, (b) input and output values expressed in metric units, although actual computations are conducted in the English system; (2) EXPLORE-I application to Grays Harbor used steady state river inflows and abbreviated subset of constituents due to data limitations; (3) Model originators: (a) EXPLORE—I derived from several unspecified water quality models by Battelle Pacific Northwest Laboratories, Richland, Washington

Table 4A-19. Summary of the Outfall Plume Model (PLUME)

Characteristic	Summary Data
Applicable Water Body	(1) Coastal waters; (2) Estuaries; (3) Lakes
Water Body Characteristics	(1) Scale: (a) near field; (2) System boundaries: (a) boundaries established that correspond closely to the plume dimensions, (b) semi-infinite half-spaces frequently used; (3) Flows: (a) assumes that the receiving water body is stagnant, (b) simulates initial dilution of the effluent plume, not transport of residuals throughout the natural system, (c) simulates within stratified aquatic environment
Time Properties	(1) Time variability: (a) steady state
Space Properties	(1) Dimensionality: (a) three dimensions, horizontal plane (two dimensions) and vertical plane (one dimension); (2) Discretization limits: (a) model permits up to 50 layers
Physical Processes	(1) Principal driving forces: (a) discharge momentum, (b) buoyancy-water density differences; (2) Processes represented: (a) dilution of effluent discharge, (b) turbulent mixing; (3) System hydrodynamics: (a) simulates behavior of a buoyant, round effluent plume being discharged into nonflowing water body, (b) considers density differences between freshwater (with residuals) and saltwater masses
Chemical Processes	(1) Processes represented: (a) considers only unspecified conservatives
Ecological Processes	(1) None
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) similarity solution
Input Data Requirements	(1) Initial setup/calibration: (a) water temperature profile (with depth), (b) salinity or density profile (with depth), (c) effluent flow rate, (d) effluent density, (e) outfall port diameter, number of discharge points, depth of discharge points, angle of discharge points to horizontal plane; (2) Verification: (a) initial constituent concentrations throughout the plume
Ease of Application	(1) Model documentation: (a) documentation report available from EPA Environmental Research Lab, Corvallis, Oregon; (2) Documentation contents: (a) adequate for most applications, (b) contains few subroutine descriptions, comment statements, or other information relevant to program modification; (3) Modifications: (a) minimal number of card changes necessary to change program, (b) recomputation time very short for modifications
Output and Output Format	(1) Output information: (a) labeled input values, (b) constituent dilution along the plume centerline, (c) depth at which plume stabilizes; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) PLUME cannot be directly linked to far field models to transport discharged residuals through the system
Manpower Needs	(1) Requires one computer programmer or one hydraulics engineer with programming experience; (2) Previous experience in FORTRAN programming useful, but model fairly simple to use
Costs	(1) Model acquisition: (a) nominal charge, e.g., less than $10, for documentation reports from EPA Environmental Research Lab, Corvallis, Oregon; (2) Model setup and data preparation: (a) up to one man-week necessary; (3) Actual computation: (a) ranges between one and three dollars per simulation run; (4) Output analysis: (a) only one or two man-hours
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes no water flow other than plume-induced movement, (b) neglects decay of residuals discharged; (2) Accuracy: (a) solution technique presents no dispersion or stability problems; (3) Sensitivity: (a) sensitive to discharged fluid density and flow rate, (b) sensitive to extent of stratification, (c) sensitive to physical features of outfall--diameter of openings, number of ports, and port depth
Other Comments	(1) PLUME developed by EPA Environmental Research Lab to assist in ocean outfall design; (2) Limitations: (a) model does not simulate transport of discharged residuals by mechanisms other than mixing and dilution of fluids with different densities, (b) model lacks advective transport, tidal dispersion, and decay of discharged constituents, (c) PLUME will not handle negatively-buoyant flows discharged with upward momentum

Table 4A-20. Summary of the Estuary Hydrodynamic/Salinity Model (HYD/SAL)

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries semi-enclosed by barrier islands; (2) Nearshore coastal waters
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) shallow water body divided into square areal grids, (b) internal system boundaries to flow considered; (3) Flows: (a) considers freshwater inputs and ocean tides; (4) Morphology: (a) square grids do not correspond exactly to irregular shorelines, (b) islands, reefs, and spoil banks handled as partial internal boundaries, (c) inundation of tidal flats and marshes by high tide usually occurs outside of the model grid, (d) handles only unstratified systems
Time Properties	(1) Time variability: (a) dynamic, (b) steady state option available; (2) Time units of application: (a) computational time steps in minutes to ensure hydrodynamic model stability, but salinity model utilizes time steps of 5-25 hours, (b) weather data input at three hour intervals, (c) bay inflow conditions established as monthly or seasonal averages
Space Properties	(1) Dimensionality: (a) two dimensions, horizontal plane; (2) Discretization limits: (a) rectangular grid can have variable-sized cells reflecting available data base and stability balance with computation time step, (b) one mile square grids common
Physical Processes	(1) Principal driving force: (a) tidally-induced convection; (2) Processes represented: (a) convection, (b) dispersion, (c) dilution, (d) evaporation, (e) wind stress, (f) Coriolis acceleration
Chemical Processes	(1) Processes represented: (a) none; (2) Constituents represented: (a) conservative inorganics only, i.e., salinity-chlorides, total dissolved solids
Ecological Processes	(1) None
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) for hydrodynamics, explicit finite difference with time-staggered computations for x and y dimensions, (b) for salinity transport, alternating implicit formulation of finite differences
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) model developed for UNIVAC 1100 series digital computers, (b) possible to use on IBM computers if core storage is set at zero prior to execution, (c) HYD requires 35,000-41,000 word storage on UNIVAC systems, (d) SAL requires 25,000 word capacity on UNIVAC systems
Input Data Requirements	(1) Initial setup/calibration: (a) hydrogeometric data, (b) tides, (c) system depths, (d) river inflows, discharges, return flows, and other flow sources, (e) flow diversions and withdrawals, (f) Coriolis acceleration, (g) bottom roughness factor, (h) rainfall rates, (i) evaporation rates, (j) wind speed and direction, (k) initial salinity patterns, (l) adjacent coastal water salinity, (m) salinity discharges--sources, quantities, (n) dispersion coefficients; (2) Verification: (a) net water exchange rates for tidal passes, (b) time history of tidal amplitudes throughout the estuary, (c) time history of salinity concentrations throughout the estuary
Ease of Application	(1) Model documentation: (a) documentation report and associated report on evaporation considerations available from Texas Water Development Board (TWDB), (b) early theoretical descriptions available from several reports of the Hydraulic Engineering Laboratories, University of Texas, Austin, Texas, (c) no complete user's manual available that describes data deck design, subroutines, or sample application; (2) Availability of operational model: (a) HYD and SAL programs can be obtained from TWDB Systems Analysis Division; (3) Modifications: (a) smaller grid sizes require extensive monitoring program for proper calibration
Output and Output Format	(1) Output information: (a) HYD output includes time history of tidal amplitude and flow velocity and direction (net convective flow) in each computational cell, (b) SAL yields time history of salinity concentration in each computational cell; (2) Output format: (a) tabular printout, (b) time history plots, (c) magnetic tape or cards for SAL computations
Linkages to Other Models	(1) HYD produces hydrodynamic data base for use by the salinity transport model, SAL; (2) HYD hydrodynamic outputs can also be used in more complex water quality and ecologic models, such as ESTECO; (3) HYD/SAL can interface with TWDB RIVTID Model which simulates river flooding and inundation of peripheral wetlands
Manpower Needs	(1) Requires computer programmer and experienced hydraulic engineer; (2) Previous experience in estuarine hydrodynamics useful; (3) Coordinated monitoring program to provide verification data requires extensive field effort by hydrologists, engineers, water chemists, and others
Costs	(1) Model acquisition: (a) preliminary HYD/SAL documentation reports available at nominal cost from Texas Water Development Board, Austin, Texas, (b) model programs operational for several Texas estuaries and available from TWDB; (2) Model setup and data preparation: (a) extensive data base required for calibration/verification, cost variable depending on estuary being studied; (3) Actual computation: (a) $10-20 per tidal cycle depending on estuary size; (4) Output analysis: (a) preparation of graphs, time history plots, and isopleth maps may require several man-hours for each simulation run

Table 4A-20. HYD/SAL (continued)

Characteristic	Summary Data
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes that estuarine water is unstratified and vertically well-mixed, (b) assumes tidally-generated convection in either direction can be represented with vertically integrated velocities, (c) neglects peripheral estuarine areas affected by tidal inundation, i.e., marshes and tidal flats; (2) Accuracy: (a) stability affected by relationship between size of computation cells and prescribed time steps; (3) No information available on model sensitivity to input parameters
Other Comments	(1) HYD/SAL developed for Texas Water Development Board by Frank D. Masch and Associates (presently Water Resources Engineers, Austin); (2) Model limitations: (a) requires extensive data base collected especially for the prototype system being modeled, i.e., sampling locations corresponding to model computation cells

Table 4A-21. Summary of the Modified River Quality Model (QUAL-II)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Man-made converging water conveyance structures
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) handles longitudinal boundaries only; (3) Flows: (a) only constant inflows and point source discharges considered, (b) each stream segment is considered instantaneously well-mixed; (4) Morphology: (a) mainstem river may have several tributary branches
Time Properties	(1) Time variability: (a) quasi-steady state--constant inflows and residuals discharges but variable meteorology; (2) Time units of application: (a) one-day time steps
Space Properties	(1) Dimensionality: (a) one dimension, horizontal plane; (2) Discretization limits: (a) up to 75 reaches, 90 point discharges, 15 junctions, (b) no length limitations on stream segments (one mile units common)
Physical Processes	(1) Principal driving force: (a) net downstream flow; (2) Processes represented: (a) dilution, (b) advection, (c) dispersion, (d) heat budget
Chemical Processes	(1) Processes represented: (a) BOD-DO reactions coupled, (b) other reactions uncoupled; (2) Constituents: (a) BOD, (b) DO, (c) ammonia, (d) nitrate, (e) nitrite, (f) temperature, (g) phosphorus, (h) benthic oxygen demand, (i) radioactive substances, (j) 3 conservative constituents (user's option); (3) Temperature effects and reaeration important to chemical reactions
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) first-order microbial decay, (c) algal growth; (2) Trophic levels: (a) only primary producers and decomposers represented; (3) Water quality-biota relationships represented: (a) algal-nutrient interactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, numerical integration
Computation Status	(1) Model coded in Fortran IV (G level); (2) Equipment requirements: (a) digital computer with 45,000 word storage capacity, (b) Fortran IV compiler
Input Data Requirements	(1) Initial setup/calibration: (a) headwater flows and distributed inflows, (b) discharges and withdrawals (constant), (c) stream depth, width, and bottom roughness, (d) concentrations of water quality consitutents at headwaters (constant), (e) residuals discharges (flow and concentration constant), (f) BOD decay and other decay rates, (g) weather conditions and evaporation coefficients; (2) Verification: (a) flows throughout the modeled area, (b) concentrations of water quality constituents throughout the modeled area
Ease of Application	(1) Model documentation: (a) documentation report available from EPA Planning Assistance Branch or Water Resources Engineers, Walnut Creek, Calif.; (2) Documentation contents: (a) good theory discussion and helpful subroutines; (3) Modifications: (a) card changes necessary only for weather conditions, (b) recomputation time for data deck changes sort
Output and Output Format	(1) Output information: (a) concentrations of water quality parameters in each reach at specified timesteps, (b) final concentrations at end of simulation, (c) average reach coefficient used in each simulation; (2) Output format: (a) tabular printout
Linkages to Other Models	(1) Model cannot handle nonpoint discharges except as steady state distributed inputs; (2) QUAL-II may be linked to more complex ecologic submodel, but currently no biotic effects above the primary producer level possible
Manpower Needs	(1) Requires one computer programmer or one environmental engineer with programming experience; (2) Previous experience in water quality models based on Fortran IV useful
Costs	(1) Model acquisition: (a) not over $25 for reproduction of the original report, because it is no longer available; (2) Model setup and data preparation: (a) 4-10 man-weeks; (3) Actual computation: (a) $10-75 per run, depending upon system discretization and number of water quality constituents
Model Accuracy and Sensitivity	(1) Representativeness: (a) handles only constant flows and discharges, (b) does not consider variations with depth or within stream cross-section; (2) Accuracy: (a) unconditionally stable, (b) low dispersion; (3) Sensitivity: (a) known values--high for depth and weather, low for initial conditions, headwater temperatures, and friction coefficient, (b) estimated values--high for wasteloads and flow velocities, decay rates, settling coefficients, low for reaeration coefficient
Other Comments	(1) QUAL-II developed by Water Resources Engineers, Walnut Creek, Calif. for Environmnetal Protection Agency; (2) Model is a modification of QUAL-I which adds eight more water quality constituents; (3) Model has a flow augmentation option

Table 4A-22. Summary of the Lake Ecologic Model (LAKECO)

Characteristic	Summary Data
Applicable Water Body	(1) Lakes; (2) Reservoirs
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) handles vertical variation in chemical, biological, and thermal parameters for well-stratified water bodies; (3) Morphology: (a) reservoir or lake should not have major arms, (b) Froude number should be less than 0.3
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) simulation time steps usually one day or less (3 hrs. common), (b) meteorology and quantity/quality inputs may be altered every three hours
Space Properties	(1) Dimensionality: (a) one dimension, vertical plane; (2) Discretization limits: (a) less than 100 layers, (b) up to 10 inflows and 10 lake outlets
Physcial Processes	(1) Processes represented: (a) advection, (b) diffusion, (c) dilution, (d) heat budget, (2) Temperature effects on various rate functions considered
Chemical Processes	(1) Processes represented: (a) over 20 intercoupled chemical and biological reactions; (2) Constituents represented: (a) DO, (b) BOD, (c) pH, (d) carbon dioxide, (e) alkalinity, (f) ammonia, (g) nitrite, (h) nitrate, (i) total dissolved solids, (j) total carbon, (k) organic detritus, (l) temperature, (m) toxicity (unspecified)
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) growth, (c) respiration, (d) mortality, (e) decay, (f) benthic nutrient regeneration; (2) Trophic levels represented: (a) decomposers--coliform, (b) primary producers--algae, (c) herbivores--zooplankton, (d) consumers--fish, benthos; (3) Water quality-biota relationships respresented: (a) algae-nutrient relationships, (b) fish toxicity relationships
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) core storage capacity of 50,000 words, (b) one tape or disk, (c) previous applications have utilized IBM 370, IBM 360, CDC 6600, and UNIVAC 1108 systems
Input Data Requirements	(1) Initial setup/calibration: (a) flow rate for all lake inflows, (b) surface area and volume relationships with lake depth (usually presented in tabular form), (c) outflow locations, (d) lake latitude and longitude, (e) concentrations of quality constituents and temperatures in all lake inflows over the simulation period, (f) initial concentrations of quality constituents and temperatures in each lake layer, (g) all kinetic parameters for each layer, including growth rates, respiration rates, (h) light extinction coefficient, (i) temperature stability coefficient, (j) diffusion coefficients, (k) meteorological data--daily wind speed and direction, air temperatures (dry and wet bulb), sky cover, atmospheric pressure; (2) Verification: (a) vertical profile of concentrations of water quality constituents and temperatures during the simulation period, (b) constituent concentrations and temperatures at the lake outflow for several time periods, (c) time history of water surface elevation during the simulation period
Ease of Application	(1) Model documentation: (a) model documentation and program listings available from the Department of Interior, Office of Water Resources Research, Washington, D.C., (b) initial report on Lake Washington application documents model theory well; (2) Difficulty: (a) large size of input decks may require considerable time for setup; (3) Modifications: (a) few card changes needed except for weather conditions, (b) recomputation time short following card changes
Output and Output Format	(1) Output information: (a) time history of temperature and constituent concentrations in each lake layer, (b) time history of temperature and constituent concentrations in each lake outflow, (c) all input values; (2) Output format: (a) tabular printout, (b) magnetic tape for system hydrodynamics
Linkage to Other Models	(1) Lake outflows may be linked to downstream river quality models; (2) Nonpoint source residuals inputs can be estimated from drainage basin size and input into the lake model
Manpower Needs	(1) Requires elementary programmer and experienced water quality engineer to apply model and set up large data deck; (2) Additional experience in analyzing biological relationships helpful to establish appropriate ecological relationships
Costs	(1) Model acquisition: (a) nominal cost for documentation reports and program listings from Dept. of the Interior, Office of Water Resources Research and NTIS, Springfield, Va.; (2) Model setup and data preparation: (a) 6 to 18 man-weeks may be necessary to get the model through the verification stage; (3) Actual computation: (a) ranges from $30-100 depending upon the complexity of the system, length of simulation period, and the number of constituents being simulated; (4) Output analysis: (a) several man-hours necessary to evaluate each simulation run
Model Accuracy and Sensitivity	(1) Representativeness: (a) neglects horizontal variations in water movement, temperature, and constituent concentrations, (b) accuracy of simulation decreases if system has major arms or Froude number exceeds 0.3; (2) Sensitivity: (a) highly sensitive to temperature and temperature dependent coefficients, (b) sensitive to input conditions and kinetic parameters for fish and zooplankton
Other Comments	(1) LAKECO is a detailed ecologic simulation model originally derived from the Deep Reservoir Model; (2) Originally developed by C. W. Chen and G. T. Orlob at Water Resources Engineers for Office of Water Resources Research and applied to Lake Washington; (3) LAKECO application requires a separate meteorological data preparation program

Table 4A-23. Summary of the Estuary Ecologic Model (ECOMOD)

Characteristic	Summary Data
Applicable Water Body	(1) Non-stratified estuaries
Water Body Characteristics	(1) Scale: (a) far field; (2) Flows: (a) residuals inputs may be dynamic or steady state, (b) steady or unsteady (dynamic) flow patterns may be specified for system inflows; (3) Tides: (a) tidal movements considered as inflows at system boundaries, (b) can handle exposed mud flats at low tide and wind effects
Time Properties	(1) Time variability: (a) dynamic, (b) user has option to input steady state conditions
Space Properties	(1) Dimensionality: (a) two dimensions, horizontal plane; (2) Discretization limits: (a) channel-junction network limited to 100 channels, (b) maximum of 20 variable inflows exclusive of tides
Physical Processes	(1) Principal driving forces: (a) net flow, (b) tides; (2) Processes represented: (a) advection, (b) dilution, (c) temperature effects
Chemical Processes	(1) Processes represented: (a) a variety of intercoupled chemical reactions and chemical-biological reactions; (2) Constituents represented: (a) DO, (b) BOD, (c) total carbon, (d) ammonia, (e) nitrite, (f) nitrate, (g) phosphate, (h) carbon dioxide, (i) alkalinity, (j) detritus, (k) total dissolved solids, (l) pH, (m) toxicity
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) growth, (c) respiration, (d) mortality, (e) benthic regeneration, (f) first and second order decay, (g) coliform die-off; (2) Trophic levels represented: (a) decomposers--coliforms, (b) primary producers--algae, (c) consumers--zooplankton, benthos, fishes; (3) Water quality-biota relationships represented: (a) algal-nutrient relationships, (b) biota-toxicity effects, (c) benthos-organic carbon relationship
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) digital computer with core storage capacity of 100,000 words--50,000 words for HYDRO module and 50,000 words for ECOSIM package, (b) two tapes or disks for HYDRO and another two for ECOSIM, (c) previous applications of HYDRO and ECOSIM have been run on IBM 370/65, CDC 6600, and UNIVAC 1108 systems
Input Data Requirements	(1) Initial setup/calibration: (a) flow rate for each inflow or withdrawal, (b) widths and depths of each channel, (c) initial water surface elevations at all junctions, (d) initial flow velocities in all channels, (e) time history of tide heights at seaward boundary, (f) optional evaporation rate and average wind speed, (g) meteorological conditions--dry and wet bulb air temperature, atmospheric pressure, sky cover, wind speed and direction, (h) latitude and longitude of the prototype system, (i) initial water temperatures and concentrations of chemical and biological constituents at all junctions, (j) water temperatures and constituent concentrations in all system inflows, (k) decay rates and other kinetic parameters; (2) Verification: (a) set of observed data giving time history of water surface elevations and flow velocities throughout the system during the simulation period, (b) time history of water temperatures and constituent concentrations throughout the system during the simulation period
Ease of Application	(1) Model documentation: (a) documentation reports and program listings available from Dept. of the Interior, Office of Water Resources Research, Washington, D.C.; (2) Modifications: (a) few card changes needed except for weather conditions, (b) short recomputation time for card changes
Output and Output Format	(1) Output information: (a) time history (daily averages) of water surface elevations, channel flows, and velocities at each junction--user may specify frequency and location of outputs, (b) time history plots of water surface elevations for specified junctions, (c) time history of water temperatures and constituent concentrations at each junction for user-specified time step, (d) all input hydrologic and quality parameters; (2) Output format: (a) tabular printout, (b) plots, (c) magnetic tape
Linkages to Other Models	(1) Linkage to activity models possible because time-varying residuals inputs can be handled
Manpower Needs	(1) Requires one programmer and one experienced water quality engineer; (2) Familiarization period of several weeks helpful to programmer before model application undertaken; (3) Ecologist or engineer experienced in water quality and biological analyses can be useful in calibrating and verifying ECOMOD
Costs	(1) Model acquisition: (a) nominal charge for model documentation reports from Office of Water Resources Research, Washington, D.C.; (2) Model setup and data preparation: (a) 5 to 15 man-weeks may be necessary to get model through the verification stage; (3) Actual computation: (a) ranges between $30-120 per run depending on the size of the modeled system, length of simulation period, and number of constituents represented; (4) Output analysis: (a) several man-hours necessary to evaluate each output
Model Accuracy and Sensitivity	(1) Representativeness: (a) does not simulate diffusion, (b) trophic relationships not overly simple; (2) Accuracy: (a) stability dependent upon establishing proper interrelationships among channel length, depth, width, slope, Manning's roughness coefficient, flow, and velocity; (3) Sensitivity: (a) HYDRO module sensitive to input tide heights, large inflow quantities, and channel depth, slope, and Manning's coefficient, (b) sensitivities to quality and biological constituents unknown
Other Comments	(1) ECOMOD consists of a hydrodynamic module (HYDRO) and a quality-ecologic module (ECOSIM); (2) Hydrodynamics simulated in similar manner to estuarine version of RECEIV; (3) Successful applications of ECOMOD have been performed on San Francisco Bay and Monterey Bay, California by Water Resources Engineers (Walnut Creek, California)

Table 4A-24. Summary of the Estuarine Aquatic Ecologic Model (ESTECO)

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries; (2) Nearshore coastal waters
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) shallow (vertically-mixed) system subdivided into square grid network, (b) different grid types account for inflows, internal system barriers to flow, and water-land interfaces, (c) can account for shallow tidally-inundated marshes and flats if HYD-RIVTID combination used; (3) Flows: (a) considers net freshwater inflows and tides to describe convective transport; (4) Morphology: (a) performs best in shallow, unstratified estuaries, (b) can account for irregular shorelines, reefs, spoil banks, tidal flats, marshes, and other critical estuarine subsystems
Time Properties	(1) Time variability: (a) quasi steady state, but dynamic conditions possible; (2) Time units of application: (a) computation time interval of 1-3 minutes for hydrodynamic solution, results reported hourly, (b) time steps of less than one day predominate (e.g., six hours used in some applications)
Space Properties	(1) Dimensionality: (a) two dimensions, horizontal plane; (2) Discretization limits: (a) orthogonal grids can vary in size depending on size of prototype system, but specified size to be uniform for all cells, (b) one square mile grids common for applications to several Texas estuaries
Physical Processes	(1) Principal driving force: (a) tidally-induced convection (net flows); (2) Processes represented: (a) convection, (b) dispersion, (c) dilution, (d) evaporation, (e) wind stress, (f) Coriolis acceleration
Chemical Processes	(1) Processes represented: (a) wide variety of predominately coupled chemical interactions; (2) Constituents represented: (a) DO, (b) BOD, (c) total dissolved solids, (d) total inorganic carbon, (e) alkalinity, (f) total phosphates, (g) ammonia nitrogen, (h) nitrites, (i) nitrates, (j) pH, (k) detritus, particulate organics, organic sediment
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) respiration, (c) biological decay, (d) benthic uptake and release, (e) mortality, (f) coliform die-off, (g) migration, (h) harvest, (i) excretion; (2) Trophic levels represented: (a) primary producers--phytoplankton, (b) herbivores--zooplankton, (c) higher consumers--bottom feeding fish, planktivorous fish, piscivorous fish, (d) decomposers--benthic animals (detritus and organic sediment feeders), coliform bacteria; (3) Water quality-biota relationships represented: (a) algal-nutrient interactions, (b) detritus-benthos and fish interactions, (c) possibility of biota-toxicity effects by differential mortality rates
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) equations for individual constituents solved via finite difference, (b) concentration in each computational cell calculated by alternating direction implicit numerical solution
Computational Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) computer storage required varies with number of computation cells representing prototype, e.g., approximately 50,000 words on UNIVAC 1100 series needed for San Antonio Bay with 380+ grid network, (b) magnetic tape for HYD output before interfacing with ecologic module
Input Data Requirements	(1) Initial setup/calibration: (a) system geometry, (b) bathymetry, (c) bottom roughness, (d) freshwater inflow rates, (e) residuals discharges, (f) system withdrawals and diversions, (g) rainfall rates, (h) evaporation rates, (i) steady wind conditions, (j) tide data, (k) kinetic parameters, including chemical reaction rates and biological activity rates, (l) dispersion coefficients, (m) initial concentrations of quality constituents and biological components from river inflows, residuals discharges, and coastal water exchange, (n) solar radiation; (2) Verification: (a) water surface elevations and velocities throughout the prototype system for several tidal periods, (b) observations of quality constituent concentrations, biological components and temperatures at various points throughout the prototype system
Ease of Application	(1) Model documentation: (a) program documentation and user's manual available from Texas Water Development Board (TWDB), Austin, Texas; (2) Documentation contents: (a) useful report presents theoretical basis, program listings, subroutine identification, data deck design, and sample model application, (b) user's manual should be augmented with HYD/SAL hydrodynamics documentation report; (3) Availability of operational model: (a) ESTECO programs for several Texas estuaries can be obtained through TWDB Systems Analysis Division, (4) Difficulties: (a) dynamic migrations of estuarine populations require extensive monitoring program, (b) large-scale field monitoring program needed to obtain tidal exchange data at coastal passes; (5) Modifications: (a) documentation report illustrates procedure for card changes, (b) model recomputation time short after card changes
Output and Output Format	(1) Output information: (a) initial input values, (b) time history of constituent concentrations, temperatures, and biological components throughout the system, (c) data from selected computation cells, (d) output on specified constituents throughout the system, (e) specialized biological outputs such as component carbon (biomass) values and productivity/respiration relationships; (2) Output format: (a) tabular printout, (b) magnetic tapes or punched cards for hydrodynamic outputs
Linkages to Other Models	(1) ESTECO receives its hydrodynamic inputs from Texas Water Development Board HYD/SAL and/or RIVTID before simulating quality conditions and ecologic parameters for the estuary; (2) Residuals input can be handled if appropriate computation cells are provided for input points

Table 4A-24. ESTECO (continued)

Characteristic	Summary Data
Manpower Needs	(1) Requires one computer programmer and/or experienced hydraulic engineer to produce hydrodynamic solution; (2) Interdisciplinary effort necessary to simulate complex estuarine ecological relationships, e.g., estuarine ecologist, water quality engineer, ocean engineer; (3) Previous experience in ecologic-water quality modeling and estuarine hydrodynamics preferred
Costs	(1) Model acquisition: (a) documentation report available without charge from Texas Water Development Board, Austin, Texas; (2) Model setup and data preparation: (a) extensive monitoring effort needed to supply input, calibration, and verification data, (b) 3 to 4 man-months may be required for setup/verification; (3) Actual computation: (a) about $60 for 2 month simulation of large bay system; (4) Output analysis: (a) review of a complete system simulation may take several man-hours, but optional single cell or single constituent outputs may reduce time required for output analysis
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes that estuary is unstratified and vertically well-mixed, (b) hydrodynamic module assumes that tidally-induced convection in either direction can be represented with vertically-integrated velocities, (c) HYD and RIVTID combination allows simulation of estuarine areas, e.g., marshes and tide flats, not included in the computational grid, (d) computations for fish carried out for the entire system, so averaged output value neglects migrations within the estuary; (2) Accuracy: (a) stability affected by relationship between size of computation cells and prescribed time step; (3) Sensitivity: (a) no information on sensitivity to various input parameters provided in documentation report
Other Comments	(1) Model hydrodynamics derived from HYD and RIVTID models, ecologic components similar to those in LAKECO; (2) ESTECO developed for Texas Water Development Board by Water Resources Engineers, Austin, Texas; (3) Extensive monitoring program required to provide basic data for steady state solution, data requirements for dynamic solution even greater

Table 4A-25. Summary of the Lake Phytoplankton Model (LAKE-1)

Characteristic	Summary Data
Applicable Water Body	(1) Freshwater lakes
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) can handle stratified, three-layer system, (b) assumes mixed horizontal dimension with vertical gradients; (3) Morphology: (a) epilimnion extends from surface to 17m depth, hypolimnion occurs between 17m and 90m depth, benthos extends from 90m to actual bottom (if shallower than 90m, last 0.5 feet used as benthos)
Time Properties	(1) Time variability: (a) steady state, e.g., residuals inputs constant for each solution; (2) Time units of application: (a) time steps of 0.5 days used, (b) data inputs and outputs are monthly averages, initial conditions start in January
Space Properties	(1) Dimensionality: (a) one dimension, vertical axis; (2) Discretization limits: (a) data generally given for 3 layers, but 67 layers at various depths are possible in later versions
Physical Processes	(1) Principal driving forces: (a) horizontal transport, (b) vertical dispersion between layers, (c) lake inflows-lake outflow (inflows split proportionally between layers); (2) Processes represented: (a) advection and diffusion to provide circulation pattern, (b) thermocline established by setting vertical dispersion between layers to zero and seasonal overturns simulated by variable vertical mixing rates
Chemical Processes	(1) Processes represented: (a) both coupled and uncoupled reactions; (2) Constituents represented: (a) dissolved CO_2--carbonate buffer system, (b) temperature, (c) pH, (d) nitrogen--organic N, ammonia, nitrate, (e) phosphorus--organic P, ortho P, (f) organic carbon--zooplankton and upper trophic level biomass
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) growth, (c) decay, (d) respiration, (e) algal-zooplankton dynamics (grazing important), (f) higher consumer relationships (relatively simple); (2) Water quality-biota relationships represented: (a) algal-nutrient interactions
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference, numerical integration
Computation Status	(1) Model coded and operational in FORTRAN IV; (2) Equipment requirements: (a) currently being run on CDC 6600, (b) new version to be available on Optimal Systems, Inc. equipment
Input Data Requirements	(1) Initial setup/calibration: (a) average depth for 4 km^2 grids, (b) water temperature variation with depth, (c) solar radiation and photo-period, (d) water clarity, (e) nutrient inputs as mass loadings (mass/unit time) or boundary conditions (mass/unit volume), (f) initial conditions for phytoplankton, zooplankton, and consumer biomass; (2) Verification: (a) observed concentrations of chlorophyll α, primary production (mg C/m^2/day), total zooplankton carbon, bottom deposition rate (mg C/m^2/year), phosphorus, orthophosphorus, total Kjeldahl nitrogen, ammonia, nitrate
Ease of Application	(1) Model documentation: (a) documentation report available as EPA 660/3-75-005, from GPO or NTIS; (2) Documentation contents: (a) report contains model theory and verification results; (3) Source listings and sample inputs-outputs available from EPA Grosse Ile Lab., Gross Ile, Michigan
Output and Output Format	(1) Output information: (a) average phytoplankton biomass per month for a one year simulation, (b) nutrient pools and zooplankton biomass also available as monthly averages, (c) outputs at 0.5 day time steps also possible; (2) Output format: (a) printed tabular format (can yield digital overplots), (b) tape outputs (can yield 3-dimensional plots or visual projections)
Linkages to Other Models	(1) Model can be linked to LAKE-2 (7-layer model) or LAKE-3 (67 segment, coarse-grid model); (2) Mass loadings of nutrients via atmospheric fallout might be possible
Manpower Needs	(1) Requires computer programmer or environmental engineer with programming experience; (2) Experience in water quality models based on FORTRAN IV helpful; (3) Data collection should involve ecologist or limnologist
Costs	(1) Model acquisition: (a) $7.00 for NTIS report, (b) charge for source listing and test runs from EPA unknown; (2) Model setup and data preparation: (a) man-days to reduce stored and limnological cruise data are unknown; (3) Actual computation: (a) actual execution time for one year simulation = 7 CPU seconds, (b) total CPU time = 30 seconds for one year simulation, (c) originators converted overhead to equivalent of 115 seconds per run, (d) at least 8 to 16 annual runs needed to reach steady state
Model Accuracy and Sensitivity	(1) Representativeness: (a) adequately represents nutrients and phytoplankton in the open lake, (b) later versions can handle eutrophication problems in specific lake shoreline areas; (2) Accuracy: (a) no problems reported; (3) Sensitivity: (a) model sensitive to variable vertical mixing rates, phytoplankton settling velocity, nutrient half-saturation values--which vary with species, herbivore grazing rates
Other Comments	(1) Model originated by Thomann, Di Toro, Winfield, and O'Connor, Department of Civil Engineering, Manhattan College, Bronx, New York for EPA Grosse Ile Lab., Michigan; (2) New versions, LAKE-2 and LAKE-3, can handle water-sediment interactions and horizontal distributions of phytoplankton, zooplankton, and nutrients

Table 4A-26. Summary of the Water Quality in River-Reservoir Systems Model (WQRRS)

Characteristic	Summary Data
Applicable Water Body	(1) Streams; (2) Rivers; (3) Reservoirs; (4) Lakes
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) model simulates an interconnected series of multi-layered reservoirs and river segments, (b) rivers have longitudinal boundaries, (c) reservoirs divided into layers throughout the lake depth; (3) Flows: (a) inflows into stratified reservoir enter layer with analogous water density, (b) reservoir outflows may be from stratified or well-mixed system
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) time units variable depending on set of constituents represented, but must equal or exceed one hour, (b) weather conditions may be input at 3-hour intervals, (c) simulation time steps of one day common
Space Properties	(1) Dimensionality: (a) reservoirs--one dimension, vertical plane, (b) river segments--one dimension, horizontal plane; (2) Discretization limits: (a) 100 layers per reservoir, (b) 10 tributary inflows per lake, (c) 10 inflow points per river segment, (d) six different channel cross-sections, (e) no limitations on the number of reservoirs or river reaches, (f) reservoir layers should by 1-3 meters thick
Physical Processes	(1) Principal driving force: (a) net flow (reservoir inflows distributed on the basis of temperature-dependent water density); (2) Processes represented: (a) advection, (b) diffusion, (c) dilution, (d) heat budget; (3) Temperature effects on water densities and various kinetic parameters considered
Chemical Processes	(1) Processes represented: (a) both coupled and uncoupled reactions; (2) Constituents represented: (a) BOD, (b) organic detritus, (c) organic sediment, (d) total carbon, (e) phosphate, (f) ammonia, (g) nitrites, (h) nitrates, (i) DO, (j) pH, (k) total alkalinity, (l) total dissolved solids, (m) carbon dioxide
Ecological Processes	(1) Processes represented: (a) photosynthesis, (b) temperature-varying growth, (c) respiration, (d) mortality, (e) decay, (f) benthic regeneration, (g) particulate settling, (h) harvest by man; (2) Trophic levels represented: (a) moderately complex trophic dynamics structure, (b) primary producers represented by two algal species with different optimal growth rates, (c) herbivores represented by zooplankton component, (d) decomposer compartment not represented, although coliform bacteria present, (e) consumer categories simulated by fish (3 different species) and benthic animals (unclassified); (3) Water quality-biota relationships represented: (a) algal-nutrient light interactions, (b) particulate carbon-detritus-sediment-benthos links, (c) food web mass transfers
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) 50,000 word storage capacity on UNIVAC 1108, (b) can be successfully run on UNIVAC 1108, IBM 360/50, CDC 7600, and Honeywell 600 series
Input Data Requirements	(1) Initial setup/calibration: (a) flow rates for all lake and stream inflows, (b) lake and stream hydrogeometric data, (c) lake outflow elevations and locations, (d) latitude and longitude of prototype systems, (e) Secchi disc depth for light extinction, (f) concentrations of quality constituents and biological parameters, and temperatures in all lake inflows and river segments throughout the simulation period, (g) initial conditions of quality constituents, biological parameters, and temperatures in each lake layer and river segment, (h) all kinetic parameters, including growth rates, decay rates, respiration rates, settling velocities, mortality rates, and other chemical-ecologic reactions rates, (i) temperature stability coefficients, (j) meteorological data--air temperature (wet and dry bulb), atmospheric pressure, wind speed and direction, sky cover; (2) Verification: (a) conditions of quality constituents, biological parameters, and temperatures during the simulation period (vertical profile for lakes, horizontal profile for river segments), (b) constituent concentrations, biological parameters, and temperatures at the lake outflow for specified time periods, (c) time history of lake water surface elevations during simulation
Ease of Application	(1) Model documentation: (a) documentation reports and source decks available from U.S. Army Corps of Engineers, Hydrologic Engineering Center, Davis, California; (2) Documentation contents: (a) model theory, data deck design, subroutine descriptions, and sample application; (3) Modifications: (a) few card changes required except for meteorology or flows, (b) little recomputation time necessary for changes; (4) Optional data editor program available to improve input data quality and reduce data preparation time
Output and Output Format	(1) Output information: (a) time history of quality constituents, temperatures, and biological parameters in each lake layer and river segment, (b) time history of quality constituents, temperatures, biological parameters in lake outflows, (c) all input values; (2) Output format: (a) tabular printout, (b) reservoir outflows to river system may be recorded on cards or magnetic tape
Linkages to Other Models	(1) Lake outflows provide direct inflows to downstream river quality models; (2) Outflow from each river segment provides input into the next segment or reservoir
Manpower Needs	(1) Requires computer programmer and experienced water quality engineer; (2) Additional experience and expertise in biology and water chemistry needed to establish proper ecological relationships; (3) Previous experience in detailed water quality models useful because of the potentially large data base needed for WQRRS

Table 4A-26. WQRRS (continued)

Characteristic	Summary Data
Costs	(1) Model acquisition: (a) documentation report costs less than $5 from the Hydrologic Engineering Center, Davis, California, (b) complete computer programs can be obtained from HEC for $60; (2) Model setup and data preparation: (a) 6 to 18 man-weeks, depending upon the data base size and utilization of the optional data editor program; (3) Actual computation: (a) ranges from $30-100 per run, depending upon the system size and extent of discretization, length of simulation, and number of constituents considered; (4) Output analysis: (a) several man-hours necessary to evaluate each simulation run
Model Accuracy and Sensitivity	(1) Representativeness: (a) assumes no vertical or lateral variations in water movement or quality constituents; (2) Accuracy: (a) no stability problems reported if time steps are not set too large; (3) Sensitivity: (a) highly sensitive to temperature (flow distribution into reservoir layers) and temperature-dependent coefficients (kinetic parameters), (b) sensitive to kinetic parameters for algae, zooplankton and fish
Other Comments	(1) WQRRS is composed of LAKECO (reservoir representation), a river ecologic model, and associated subroutines; (2) Optional data editor program can improve model calibration and verification; (3) WQRRS originally developed for HEC by Water Resources Engineers for application to the Trinity River basin, Texas; (4) Future modifications will include representation of lakes with major arms and additional ecologic components, e.g., toxic materials, suspended solids, and attached algae

Table 4A-27. Summary of the Narragansett Bay Hydrodynamic Model

Characteristic	Summary Data
Applicable Water Body	(1) Estuaries; (2) Nearshore coastal waters
Water Body Characteristics	(1) Scale: (a) far field; (2) System boundaries: (a) utilizes grid network to represent x and y directions, (b) grid interfaces may be water-land and water-water; (3) Flows: (a) river inflows, residuals discharges, and tides represented by at least two boundary condition grids, (b) simulates tidal hydrodynamics (flow velocities, currents, tide heights); (4) Morphology: (a) grid network does not correspond exactly with irregular shorelines, (b) can handle irregular bathymetry, (c) stratification can be simulated by laterally-integrated quality version developed by Spaulding, but pure tidal hydrodynamics form uses vertically-averaged flow velocities
Time Properties	(1) Time variability: (a) dynamic; (2) Time units of application: (a) computation time steps in minutes, (b) output and input values usually on hourly basis
Space Properties	(1) Dimensionality: (a) two dimensions, horizontal plane; (2) Discretization limits: (a) no limits to number or size of grids specified for a given application, (b) inflow points for rivers, ocean passes, or residuals discharges must be at least two grids wide, (c) grid lengths of 0.5 nautical mile used in initial applications
Physical Processes	(1) Principal driving forces: (a) tidally-induced convection, (b) net flow if high system inflows specified; (2) Processes represented: (a) convection, (b) dispersion, (c) dilution, (d) evaporation, (e) temperature (optional)
Chemical Processes	(1) Processes represented: (a) salinity transport and simple water quality relationships available for use in association with the basic tidal hydrodynamic model; (2) Constituents represented in compatible models: (a) conservatives--salinity, (b) nonconservatives--DO, BOD, nutrients
Ecological Processes	(1) Later model versions based on the tidal hydrodynamics model can be used to simulate phytoplankton-zooplankton dynamics in Narragansett Bay
Mathematical Properties	(1) Theoretical basis: (a) deterministic assumptions; (2) Solution technique: (a) finite difference with "multi-operation" computation for basic equations--both implicit and explicit schemes involved
Computation Status	(1) Model coded in FORTRAN IV; (2) Equipment requirements: (a) currently operational on IBM 360/50, (b) magnetic tapes or disks may be required for associated transport models
Input Data Requirements	(1) Initial setup/calibration for hydrodynamic model only: (a) hydrogeometric data--system geometry, bathymetry, and boundaries, (b) initial and average depth values, (c) Coriolis factor, (d) water levels and Velocities, (e) tide data, (f) bottom roughness factor; (2) Verification: (a) time history of water levels throughout the modeled system, (b) observed current velocity data collected near the surface and near the bottom
Ease of Application	(1) Model documentation: (a) several reports outlining theoretical development and different applications available from University of Rhode Island Marine Advisory Program, Narragansett, Rhode Island; (2) Documentation contents: (a) theory, subroutines, and program listings, but reports are not complete user's manuals; (3) Modifications: (a) no information presented in reports
Output and Output Format	(1) Output information: (a) time history of water levels and flow velocity/direction for the entire system, (b) time history of water level and/or current vectors for selected portions of the computational grid; (2) Output format: (a) tabular printout, (b) numerical printouts in shape of computational grid, (c) magnetic tape or punched cards
Linkages to Other Models	(1) The Narragansett Bay tidal hydrodynamic model can be linked to a salinity transport model, DO-BOD water quality model, and nutrient-phytoplankton-zooplankton model; (2) Difficult to link model to small rivers or residuals discharges due to two-cell minimum for system inflows
Manpower Needs	(1) Requires computer programmer and experienced hydraulic engineer; (2) Previous experience in ocean engineering and estuarine hydrodynamics helpful
Costs	(1) Model acquisition: (a) documentation reports available for nominal costs, e.g., less than $5, from University of Rhode Island Marine Advisory Service; (2) Model setup and data preparation: (a) extensive monitoring effort needed to supply input, calibration, and verification data--no man-hour estimates available; (3) Actual computation: (a) no information available; (4) Output analysis: (a) no man-hour estimates available
Model Accuracy and Sensitivity	(1) Representativeness: (a) computation scheme requires at least two grids for any system inflow, (b) computation grid network neglects many marshes and shallow tide flats along irregular shorelines; (2) Accuracy: (a) model unconditionally stable, but time step increment may affect model accuracy if improperly assigned; (3) Sensitivity: (a) sensitivity experiments conducted, but results not reported
Other Comments	(1) Narragansett Bay tidal hydrodynamic model developed by K. W. Hess and F. M. White, Department of Ocean Engineering, University of Rhode Island; (2) Model has application for simulation of high freshwater inflows (non-tidal flow), current vectors and tidal co-range patterns, and hurricane storm surges; (3) Additional simulation work on salinity transport, temperature, water quality constituents, and phytoplankton-zooplankton dynamics being conducted by University of Rhode Island investigators using hydrodynamic model as foundation of research

Appendix B

REFERENCES FOR RECEIVING WATER MODELS

Streeter-Phelps Dissolved Oxygen Equation

Streeter, H. W. and E. B. Phelps. 1925. *A Study of the Pollution and Natural Purification of the Ohio River*, Public Health Bulletin 146 (Washington, D.C., U.S. Public Health Service).

Hung, J. Y., A. Hossain, and T. P. Chang. 1976. "Stream Modeling and Waste Load Allocation," in *Proceedings of the EPA Conference on* Environmental Modeling and Simulation (Cincinnati, Ohio, Environmental Protection Agency, April) pp. 129-132.

Lumped Parameter Nutrient Budget Model

Dillon, P. J. 1975. *The Application of the Phosphorus-Loading Concept to Eutrophication Research*, Scientific Series No. 46 (Burlington, Ontario, Canadian Center for Inland Waters).

Vollenweider, R. A. and P. J. Dillon. 1974. *The Application of the Phosphorus Loading Concept to Eutrophication Research*, report to Associate Committee on Scientific Criteria for Environmental Quality, Burlington, Ontario.

Long-Term Phosphorus Balance Model

Kimmel, L. V., R. G. Baca, and W. C. Weimer. 1975. *A Phosphorus Balance Model for Long-Term Prediction of Eutrophication in Lakes and Impoundments*, Report prepared by Battelle Pacific Northwest Laboratories, Richland, Washington, for U.S. Environmental Protection Agency, Office of Research and Development, Washington, D.C.

Weimer, W. C., H. E. McGuire, and A. F. Gasperino. 1976. *A Review of Land Use Nutrient Loading Rate Relationships*, Report prepared by Battelle Pacific Northwest Laboratories, Richland, Washington, for U.S. Environmental Protection Agency, Office of Research and Development, Washington, D.C.

Segmented River Dissolved Oxygen Model

O'Connor, D. J. 1960. "Oxygen Balance of an Estuary," *Journal of Sanitary Engineering Division, Proceedings of the American Society of Civil Engineers* vol. 86, no. SA3 (May) pp. 35-55.

Editors' note:
Annotations are provided only for references for models which have been summarized.

O'Connor D. J. 1967. 'The Temporal and Spatial Distribution of Dissolved Oxygen in Streams," Water Resources Research vol. 3, no. 1, pp. 65-79.

Thomann, R. V. 1963. "Mathematical Model for Dissolved Oxygen," Journal of Sanitary Engineering Division, Proceedings of the American Society of Civil Engineers vol. 89, no. SAS (October) pp. 1-30.

SNSIM

Braster, R. E., S. C. Chapra, and G. A. Nossa. 1975. Documentation for SNSIM 1/2: A Computer Program for the Steady State Water Quality Simulation of a Stream Network (4th ed., New York, U.S. Environmental Protection Agency, Region II, Systems Analysis Section).

SSM/SEM

Hydroscience, Inc. 1971. Simplified Mathematical Modeling of Water Quality, GPO 1971-444-367/392 (Washington, D.C., U.S. Environmental Protection Agency, Office of Water Programs).

This report presents the desk top analytical procedures needed to address water quality with the Simplified Stream Model and Simplified Estuary Model. Nomographs included in this report are essential to the solution methodology.

Hydroscience, Inc. 1972. Addendum to Simplified Mathematical Modeling of Water Quality, GPO 1972-484-486/291 (Washington, D.C., U.S. Environmental Protection Agency, Office of Water Programs).

This report updates certain components of the simplified modeling system for easier application.

DOSAG-I

Texas Water Development Board. 1972. DOSAG-I - Simulation of Water Quality in Streams and Canals: Program Documentation and Users Manual (Austin, Texas, Systems Engineering Division).

DOSAG-3

Duke, J. H., Jr. and F. D. Masch. 1973. Computer Program Documentation for the Stream Quality Model, DOSAG-3, Report prepared by Water Resources Engineers, Austin, Texas, for U.S. Environmental Protection Agency, Systems Development Branch, Washington, D.C., October.

This detailed documentation report describes the modifications made to the original DOSAG-I code as part of the Chattahoochee-Flint River (Georgia) Mathematical Model Project. Important user information is provided as well as descriptions of DOSAG-3 capabilities and limitations.

RIBAM

Marshall, R. N., S. G. Chamberlain, and C. V. Beckers, Jr. 1976. "RIBAM, A Generalized Model for River Basin Water Quality Management Planning," in *Proceedings of the EPA Conference on Environmental Modeling and Simulation* (Cincinnati, Ohio, Environmental Protection Agency, April).

Raytheon Oceanographic and Environmental Services. 1974a. *BEBAM - A Mathematical Model of Water Quality for the Beaver River Basin: Volume III - Documentation Report*, Report prepared for U.S. Environmental Protection Agency, Office of Water Programs, Washington, D.C.

__________. 1974b. *Expanded Development of BEBAM - A Mathematical Model of Water Quality for the Beaver River Basin*, Report prepared for the U.S. Environmental Protection Agency, Office of Water Programs, Washington, D.C.

DOSCI

Shephard, J. L. and E. J. Finnemore. 1974. *Spokane River Basin Model Project: Volume IV - User's Manual for Steady State Stream Model* (Seattle, Washington, U.S. Environmental Protection Agency, Region X).

This user's manual provides useful information concerning the set-up and application of DOSCI model for steady state water quality simulation.

Systems Control, Inc and Snohomish County Planning Department. 1974. *Water Quality Management Plan for the Snohomish River Basin and the Stillaguamish River Basin, Volume IV - Computer Program Documentation, Part A: Steady State Stream Model* (SNOSCI) (Everett, Washington, Snohomish County Planning Department).

This documentation report describes the application of DOSCI, a modification of the DOSAC-I model, to two Washington river systems.

ES001

Chapra, S. C. and S. Gordimer. 1973. *Addendum to ES001: Verification of Model for New York Harbor* (New York, U.S. Environmental Protection Agency, Region II, Data Systems Branch).

This document reviews the application of ES001 to the New York Harbor complex under summertime conditions. Specific simulation results are presented, but little information is provided for general application to other sites.

__________ and __________. 1973. *ES001: A Steady State, One-Dimensional Estuarine Water Quality Model* (New York, U.S. Environmental Protection Agency, Region II, Data Systems Branch).

This report will serve as a fairly complete documentation report and user's manual for utilizing the ES001 model. The model theory and sensitivity of important model variables are discussed in detail, as is the basic programming methodology needed to apply the model successfully.

AUTO-QUAL

Crim, R. L. and N. L. Lovelace. 1973. AUTO-QUAL Modeling System, Report No. EPA-440/9-73-003 (Washington, D.C., U.S. Environmental Protection Agency, Office of Air and Water Programs, Monitoring and Data Support Division).

QUAL-I

Texas Water Development Board. 1970. QUAL-I - Simulation of Water Quality in Streams and Canals: Program Documentation and User's Manual (Austin, Texas, Systems Engineering Division).

This initial documentation report concentrates on the QUAL-I model program and describes in detail the various program subroutines, input data needs, output files, and model flow charts. This report should be used in conjunction with the following reference (TWDB Report 128) when attempting to apply QUAL-I.

__________ and F. D. Masch and Associates. 1971. Simulation of Water Quality in Streams and Canals: Theory and Description of QUAL-I Mathematical Modeling System, Report 128 (Austin, Texas, Texas Water Development Board).

This report discussed the theoretical considerations for system hydrology, heat exchange, BOD and dissolved oxygen balance, and conservative mineral balance. It provides examples of QUAL-I application and verification on the San Antonio River (Texas).

Bansal, M. K. 1976. "Dispersion Model for an Instantaneous Source of Pollution in Natural Streams and its Applications to the Big Blue River," in Proceedings of the EPA Conference on Environmental Modeling and Simulation (Cincinnati, Ohio, Environmental Protection Agency, April) pp. 335-339.

This article discusses the theoretical development of a QUAL-I type model and its application on the Big Blue River (Nebraska).

DEM

California Water Resources Control Board. 1969. Final Report: San Francisco Bay-Delta Water Quality Control Program (Preliminary abridged ed., Sacramento, Calif., California Water Resources Control Board).

This report describes an updated DEM application to the San Francisco Bay-San Joaquin Delta estuarine system.

Feigner, K. D. and H. S. Harris. 1970. Documentation Report, FWOA Dynamic Estuary Model (Washington, D.C., U.S. Department of the Interior, Federal Water Quality Administration).

This detailed documentation report incorporated the latest developments with the Dynamic Estuary Model into a useful guide. Potential users should refer to this document for the basic characteristics of the DEM, especially the theoretical development.

Water Resources Engineers, Inc. 1965. A Water Quality Model of the San Francisco-San Joaquin Delta (San Francisco, Calif., U.S. Public Health Service, Region IX, Division of Water Supply and Pollution Control).

This report describes the original development of the DEM and application to the complex San Francisco-San Joaquin Delta.

__________. 1966. A Hydraulic Water Quality Model of Suisun and San Pablo Bays (Dallas, Texas, U.S. Department of the Interior, Federal Water Pollution Control Administration, Southwest Region).

This report describes the application of DEM to Suisun and San Pablo Bays (California).

__________. 1974a. Computer Program Documentation for the Dynamic Estuary Model (Tallahassee, Florida, Florida Department of Pollution Control).

This documentation report for the Dynamic Estuary Model details the version used in St. Andrews Bay (Florida) Water Quality Modeling Project.

__________. 1974b. Computer Program Documentation for the Dynamic Estuary Model (Washington, D.C., U.S. Environmental Protection Agency, Systems Development Branch).

This documentation report describes the DEM version used to simulate water quality in the Pearl Harbor (Hawaii) system.

__________. 1974c. Validation and Sensitivity Analyses of Stream and Estuary Models Applied to Pearl Harbor, Hawaii (Washington, D.C., U.S. Environmental Protection Agency, Systems Development Branch).

This follow-up report to the DEM application to Pearl Harbor (Hawaii) discussed validation of the model with observed water quality conditions. Sensitive DEM components are revealed through additional model testing.

TTM

Callaway, R. J. and K. V. Byram. 1971. Mathematical Model of the Columbia River from the Pacific Ocean to Bonneville Dam, Part II: Input-Output and Initial Verification Procedures (Corvallis, Oregon, Pacific Northwest Water Laboratory, U.S. Environmental Protection Agency).

This report supplements the original theory by describing actual simulated output of the TTM for the Lower Columbia River. Verification of the TTM output with observed temperatures is discussed.

__________, __________, and G. R. Ditsworth. 1969. Mathematical Model of the Columbia River from the Pacific Ocean to Bonneville Dam, Part I: Theory, Program Notes, and Programs (Corvallis, Oregon, Pacific Northwest Water Laboratory, U.S. Environmental Protection Agency).

This report presents the initial development of the Tidal Temperature Model for the portion of the Columbia River (Washington) under tidal influence. The theory and solution methodology for representing the heat budget if presented.

RECEIV

Huber, W. C., J. P. Heaney, M. A. Medina, W. A. Peltz, H. Sheikh, and G. F. Smith. 1975. Storm Water Management Model User's Manual, Version II, Report No. EPA-670/2-75-017 (Cincinnati, Ohio, U.S. Environmental Protection Agency).

This report serves as the basic user's manual for applying SWMM and its RECEIV module.

__________, __________, W. A. Peltz, S. J. Nix, and K. J. Smolenyak. 1977. "Interim Documentation, November 1977, Release of EPA SWMM." Draft, Project R-802411 (Cincinnati, Ohio, U.S. Environmental Protection Agency).

This report describes the most up-to-date version of RECEIV.

Metcalf and Eddy, Inc., University of Florida, and Water Resources Engineers, Inc. 1971. Storm Water Management Model, Volumes 1-4, EPA No. 11024DOC (Washington, D.C., U.S. Environmental Protection Agency).

This original documentation report for the Storm Water Management Model contains discussion of the Receiving Water Module (RECEIV).

RECEIV-II

Beckers, C. V., P. E. Parker, R. N. Marshall, and S. G. Chamberlain. 1976. "RECEIV-II, A General Dynamic Planning Model for Water Quality Management," in Proceedings of an EPA Conference on Environmental Modeling

and Simulation (Cincinnati, Ohio, U.S. Environmental Protection Agency, April).

Raytheon Oceanographic and Environmental Services. 1974. New England River Basins Modeling - RECEIV-II Model - Sensitivity Analysis Report (Washington, D.C., U.S. Environmental Protection Agency, Office of Water Programs).

__________. 1975. RECEIV-II - Documentation Report for Water Quantity and Quality Model, Revised report (Washington, D.C., U.S. Environmental Protection Agency, Office of Water Programs).

RIVSCI

Systems Control, Inc. and Snohomish County Planning Department. 1974a. Water Quality Management Plan for the Snohomish River Basin and the Stillaguamish River Basin: Volume III - Methodology (Everett, Washinton, Snohomish County Planning Department).

This report discusses the various mathematical models used for water quality simulation of the Snohomish and Stillaguamish River Basins, including the RIVSCI version of the Dynamic Estuary Model.

__________ and __________. 1974b. Water Quality Management Plan for the Snohomish River Basin and the Stillaguamish River Basin: Volume IV - Computer Program Documentation, Part B: Dynamic Estuary Model (SRMSCI) (Everett, Washington, Snohomish County Planning Department).

This report documents the modified version of the Dynamic Estuary Model used to simulate estuarine water quality conditions in the lower Snohomish River Basin (Washington).

WRECEV

Johnson, A. E. and J. H. Duke, Jr. 1976. Computer Program Documentation for the Unsteady Flow and Water Quality Model - WRECEV (Washington, D.C., U.S. Environmental Protection Agency, Planning Assistance Branch).

This report describes selected modifications to the RECEIV module of SWMM to make it a stand-alone model for simulating unsteady streamflow. Complete documentation is provided, including an example problem which demonstrates the methodology for successfully applying WRECEV.

DRM

Water Resources Engineers, Inc. 1967. Prediction of Thermal Energy in Streams and Reservoirs (Sacramento, Calif., California Department of Game and Fish).

This report discusses basic heat budget models, including the Deep Reservoir Model.

Water Resources Engineers, Inc. 1969a. *Mathematical Models for the Prediction of Thermal Energy Changes in Impoundments*, Publication No. EPA 16130EXT12/69 (Washington, D.C., U.S. Environmental Protection Agency, Water Quality Office).

This report details the conceptual development of the Deep Reservoir Model for temperature prediction in stratified reservoirs.

__________. 1969b. *Mathematical Models for the Prediction of Thermal Energy Changes in Impoundments - Computer Application Supplement* (Washington, D.C., U.S. Environmental Protection Agency, Water Quality Office).

This report provides some useful user information for actual application of DRM to reservoir thermal conditions.

__________. 1969c. *Temperature Prediction in Dworshak Reservoir by Computer Simulation - Computer Application Supplement* (Walla Walla, Washington, U.S. Army Corps of Engineers).

This report presents the results of simulating the heat budget in Dworshak Reservoir (Idaho) with the Deep Reservoir Model.

LAKSCI

Finnemore, E. J. and J. L. Shepherd. 1974. *Spokane River Basin Model Project: Volume I - Final Report* (Seattle, Washington, U.S. Environmental Protection Agency, Region X, Air and Water Programs Division).

This project report presents the results of water quality simulations for stratified reservoirs in the Spokane River Basin (Washington).

Shepherd, J. L. and E. J. Finnemore. 1974. *Spokane River Basin Model Project: Volume VI - User's Manual for Stratified Reservoir Model* (Seattle, Washington, U.S. Environmental Protection Agency, Region X, Air and Water Programs Division).

This user's manual describes the necessary methodology for applying the LAKSCI version of the Stratified Reservoir Model.

EPARES

Duke, J. H., Jr. 1974. Computer Program Documentation for the Reservoir Water Quality Model EPARES (Washington, D.C., U.S. Environmental Protection Agency, Systems Development Branch, January).

This detailed documentation report describes the Deep Reservoir Model and modifications made during the Chattahoochee-Flint River (Georgia) Mathematical Model Project. Essential elements of this report include theoretical considerations, basic model description, program listings and descriptions, variable descriptions, input data descriptions, and the input-output format for a sample application.

HSP

Hydrocomp, Inc. 1972a. Hydrocomp Simulation Programming: Mathematical Model of Water Quality Indices in Rivers and Impoundments (Palo Alto, Calif., Hydrocomp, Inc.).

This report discusses in detail the various water quality constituents and ecological parameters that can be simulated with HSP. The conceptual representation and solution equation(s) for each model variable are presented.

__________. 1972b. Hydrocomp Simulation Programming: Operations Manual (2nd ed., Palo Alto, Calif., Hydrocomp, Inc.).

This operations manual is intended for those persons applying the proprietary HSP model. The report describes the elements of hydrologic simulation, basic program organization, and some software programming information, but does not serve as a functional user's guide.

FEDBAK03

Chapra, S. C. and G. A. Nossa. 1974. HAR03, A Computer Program for the Modeling of Water Quality Parameters in Steady State Multidimensional Natural Aquatic Systems (New York, U.S. Environmental Protection Agency, Region II).

Nossa, G. A. 1976. "FEDBAK03, A Computer Program for the Modeling of First Order Consecutive Reactions with Feedback under a Steady State, Multi-dimensional Natural Aquatic System," in Proceedings of the EPA Conference on Environmental Modeling and Simulation (Cincinnati, Ohio, U.S. Environmental Protection Agency, April) pp. 166-170.

CAFE/DISPER

Celikkol, B. and R. Reichard. 1976. *Hydrodynamic Model of the Great Bay Estuarine System: Part I*, Report No. UNH-SG-153 (Durham, New Hampshire, Mechanics Research Laboratory, University of New Hampshire).

This report describes the use of four separate interconnecting models to represent circulation in the complex Great Bay estuarine system near Portsmouth, New Hampshire.

Pagenkopf, J. R., G. C. Christodoulou, B. R. Pearce, and J. J. Connor. 1976a. *A User's Manual for CAFE-1: A Two-Dimensional Finite Element Circulation Model*, Report 217 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology).

This detailed user's manual describes the computer software components needed to apply this hydrodynamic circulation model. Sample problems include tide and wind-induced flow in an estuary and wind-induced circulation in a lake system.

__________, __________, __________, and __________. 1976b. *A User's Manual for DISPER-1: A Two-Dimensional Finite Element Dispersion Model*, Report 218 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology).

This detailed user's manual describes the computer software components of DISPER-1. An example problem is given for a residuals discharge into a straight channel with uniform flow.

__________, __________, __________, and __________. 1976c. *Circulation and Dispersion Studies at the Pilgrim Nuclear Power Station, Rocky Point, Massachusetts*, Report 210 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology).

This report describes the application of CAFE and DISPER to simulate far field circulation and dispersion in the Massachusetts Bay region, particularly near the Pilgrim nuclear power facility.

Wang, J. D. and J. J. Connor. 1975. *Mathematical Modeling of Near Coastal Circulation*, Report MIT-SG-75-13 (Cambridge, Mass., MIT Sea Grant Program, Massachusetts Institute of Technology).

This report provides detailed information on the model development of finite element models for representing hydrodynamic circulation in coastal and estuarine systems. User-oriented information regarding the application of such models is lacking.

EXPLORE-I

Baca, R. G., W. W. Waddell, C. R. Cole, A. Brandstetter, and D. B. Cearlock. 1973. EXPLORE-I: A River Basin Water Quality Model (Richland, Washington, Battelle Pacific Northwest Laboratories).

This report discusses the initial development of EXPLORE-I, a link-node model for simulating hydrodynamics and water quality in tidally-influenced systems.

Battelle Pacific Northwest Laboratories. 1974. Development of a Mathematical Water Quality Model for Grays Harbor and Chehalis River, Washington - Documentation Report, Report No. 211B01360 to U.S. Environmental Protection Agency (Richland, Washington, Battelle Pacific Northwest Laboratories).

This report documents the application of EXPLORE-I to the tidally-influenced portions of the Grays Harbor Estuary and linkage to PIONEER-I, which simulates riverine hydrodynamics and water quality in the connecting Chehalis River. EXPLORE-I was calibrated and verified for 1970-1972 dissolved oxygen conditions.

Johnason, P. A., M. W. Lorensen, and W. W. Waddell. 1976. "A Multi-Parameter Estuary Model," in Proceedings of the EPA Conference on Environmental Modeling and Simulation (Cincinnati, Ohio, U.S. Environmental Protection Agency, April) pp. 111-114.

This brief article presents the general capabilities of EXPLORE and discusses the results of application to Grays Harbor and to the Lower Chehalis River (Washington).

SPLOTCH

Clark, P. A. A., D. J. Casey, J. P. Sandwick, and A. Solpietro. 1976. "An Empirical Model for Nutrient Accumulation Rates in Lake Ontario," in Proceedings of the EPA Conference on Environmental Modeling and Simulation (Cincinnati, Ohio, U.S. Environmental Protection Agency) pp. 176-181.

Coastal Water Quality Simulation Model

Leendertse, J. J. 1972. A Water-Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Volume IV. Jamaica Bay Tidal Flows, Pub. No. R-1009-NYC (Santa Monica, Calif., The Rand Corporation, July).

__________ and E. C. Gritton. 1971. A Water-Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Volume III. Jamaica Bay Simulations, Pub. No. R-709-NYC (Santa Monica, Calif., The Rand Corporation, July).

Leendertse, J. J. and S. Liu. 1974. A Water-Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Volume VI. Simulation, Observation, and State Estimation, Pub. No. R-1586-NYC (Santa Monica, Calif., The Rand Corporation, September).

__________ and __________. 1975a. A Water-Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Volume VII. A Hindcast, Pub. No. R-1774-NYC (Santa Monica, Calif., The Rand Corporation, July).

__________ and __________. 1975b. A Water-Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Volume VIII. An Engineering Assessment, Pub. No. R-1791-NYC (Santa Monica, Calif., The Rand Corporation, December).

MIT Lake Temperature Model

Ryan, P. J. and D. R. F. Harleman. 1971. Temperature Prediction in Stratified Water: Mathematical Model - User's Manual, Water Pollution Control Research Series 16130-DJH04/71 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology, April).

Two-Dimensional Stream Mixing Model

Bauer, D. P. and N. Yotsukura. 1974. Two-Dimensional Excess Temperature Model for a Thermally Loaded Stream, Computer Program G300 (Bay St. Louis, Miss., U.S. Geological Survey, Hydroscience Center).

Pascagoula Estuary Model

Shindala, A., V. L. Zitta, and M. W. Corey. 1973a. Water Quality Models for the Pascagoula River Basin. I. Fresh Water Streams, Report No. EIRS-CE-73-1 (Mississippi State, Miss., Engineering and Industrial Research Station, Mississippi State University).

__________, __________, and __________. 1973b. Water Quality Models for the Pascagoula River Basin. II. Tidal Estuaries, Report No. EIRS-CE-73-2 (Mississippi State, Miss., Engineering and Industrial Research Station, Mississippi State University.

Zitta, V. L., A. Shindala, and M. W. Corey. 1977. "A Two-Dimensional Mathematical Model for Water Quality Planning in Estuaries," Water Resources Research vol. 13, no. 1, pp. 55-61.

SED-II

Ariathurai, R., R. C. MacArthur, and R. B. Krone. 1977. Mathematical Model of Estuarial Sediment Transport, Technical Report D-77-12 (Vicksburg, Miss., U.S. Army Corps of Engineers, Waterways Experiment Station).

PLUME

Baumgartner, D. J. and D. S. Trent. 1970. Ocean Outfall Design: Part I, Literature Review and Theoretical Development (Washington, D.C., Federal Water Pollution Control Association).

This report reviews the application of buoyant and submerged jet plume models to simulate ocean outfall discharge.

__________, __________, and K. V. Byram. 1971. User's Guide and Documentation for Outfall Plume Model, Working Paper #80 (Corvallis, Oregon, U.S. Environmental Protection Agency, Pacific Northwest Water Laboratory).

This report provides basic user information for set-up and application of the Nearfield Outfall Plume Model.

Transient Water Quality Network Model

Harleman, D. R. F., J. E. Dailey, M. L. Thatcher, T. O. Najarian, D. N. Brocard, and R. A. Ferrara. 1977. User's Manual for the MIT Transient Water Quality Network Model, Including Nitrogen-Cycle Dynamics for Rivers and Estuaries, Pub. No. EPA-600/3-77-010 (Corvallis, Oregon, U.S. Environmental Protection Agency, Environmental Research Laboratory) and available as NTIS Publication No. PB 264-925.

Dailey, J. E. and D. R. F. Harleman. 1972. Numerical Model for the Prediction of Transient Water Quality in Estuary Networks, Technical Report 158 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology).

Najarian, T. O. and D. R. F. Harleman. 1975. A Real Time Model of Nitrogen-Cycle Dynamics in an Estuarine System, Technical Report 204 (Cambridge, Mass., Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Massachusetts Institute of Technology).

WIRQAS

Hines, W. G., D. A. Rickert, S. W. McKenzie, and J. P. Bennett. 1975. Formulation and Use of Practical Models for River Quality Assessment, Circular 715B (Reston, Va., U.S. Geological Survey).

Hines, W. G., D. A. Rickert, and S. W. McKenzie. 1976. *River-Quality Assessment of the Willamette River Basin, Oregon: Hydrologic Analysis and River-Quality Data Programs*, Circular 715-D (Reston, Va., U.S. Geological Survey).

Jennings, M. E., J. O. Shearman, and D. P. Baver. 1976. *Selection of Streamflow and Reservoir-Release Models for River-Quality Assessment*, Circular 715-E (Reston, Va., U.S. Geological Survey).

Rickert, D. A., W. G. Hines, and S. W. McKenzie. 1975. "Methods and Data Requirements for River-Quality Assessment," *Water Resources Bulletin* vol. 11, no. 5, pp. 1013-1039.

__________, __________, and __________. 1976a. *Methodology for River-Quality Assessment with Application to the Willamette River Basin, Oregon*, Circular 715-M (Reston, Va., U.S. Geological Survey).

__________, __________, and __________. 1976b. *Project Development and Data Programs for Assessing the Quality of the Willamette River, Oregon*, Circular 715-C (Reston, Va., U.S. Geological Survey).

HYD/SAL

F. D. Masch and Associates. 1971. *Tidal Hydrodynamic and Salinity Models for San Antonio and Matagorda Bays*, Texas, Report to Texas Water Development Board (Austin, Texas, Texas Water Development Board).

This report describes basic model theory and solution methodology, but lacks user-oriented information for application of this two-dimensional, orthogonal grid model. Brief descriptions of HYD/SAL Model applications to the San Antonio and Matagorda Bay systems are included.

__________. 1972. *Tidal Hydrodynamic and Salinity Models for Coastal Bays: Evaporation Considerations*, Report to Texas Water Development Board (Austin, Texas, Texas Water Development Board).

This predominantly theoretical report describes the addition of evaporation as a factor in the two-dimensional salinity transport equations. Applications of these model revisions to simulation of San Antonio Bay is discussed.

QUAL-II

Grenney, W. J., M. C. Teuscher, and L. S. Dixon. 1978. "Characteristics of the Solution Algorithms for the QUAL-II River Model," *Journal of the Water Pollution Control Federation* vol. 50, no. 1, pp. 151-157.

Useful discussion of problems in QUAL-II model application due to inherent characteristics of the solution methodology used is provided in this article.

Roesner, L. A., J. R. Monser, and D. E. Evenson. 1973. Computer Program Documentation for the Stream Quality Model, QUAL-II (Washington, D.C., U.S. Environmental Protection Agency, Systems Development Branch).

This report documents the modified QUAL-I model (QUAL-II) developed during the Iowa-Cedar River Basin (Iowa) Project. Differences in program structure for QUAL-II are explained, but the user should have access to the original QUAL-I documentation reports.

Water Resources Engineers, Inc. 1973. QUAL-II Model Validation Runs and Sensitivity Testing for the Iowa-Cedar River Basins, Report to the U.S. Environmental Protection Agency (Washington, D.C., U.S. Environmental Protection Agency, Systems Development Branch).

This report discusses the results of QUAL-II applications in the Iowa-Cedar River Basins, particularly validation of model simulations against available water quality data. Sensitivity testing of QUAL-II identified important model parameters which affect the simulated output.

LAKECO

Brandes, R. J., D. J. Glanz, and G. T. Orlob. 1973. Ecologic Simulation of Tellico Reservoir (Knoxville, Tenn., Tennessee Valley Authority).

This report describes the application of LAKECO to water quality problems in the Tellico Reservoir (Tennessee).

Gaume, A. N., R. J. Brandes, and J. H. Duke. 1975. Computer Program Documentation for the Reservoir Ecologic Model TVAECO with Tims Ford Reservoir Simulation Results (Chattanooga, Tenn., Tennessee Valley Authority, Water Quality Branch, February).

This report describes a modified version of LAKECO which was applied to the Tims Ford Reservoir on the Elk River (Tennessee). Simulation results based on 1973 data are presented along with a useful user's guide.

Water Resources Engineers, Inc. 1973. Ecologic Study of Lake Koocanusa-Libby Dam, Report to the U.S. Army Corps of Engineers (Seattle, Wash., U.S. Army Corps of Engineers, Region X).

This report discusses the application of LAKECO to Lake Koocanusa (Washington).

__________. 1975. Lake Ecologic Model User's Manual - LAKECO Ecologic Modeling, Report to U.S. Environmental Protection Agency and U.S. Department of the Interior (Washington, D.C., Office of Water Resources Research).

This user's manual presents the necessary documentation for applying the Lake Ecologic Model to a wide variety of lakes and impoundments.

EPAECO

Gaume, A. N. and J. H. Duke, Jr. 1975. Computer Program Documentation for the Reservoir Ecologic Model EPAECO (Washington, D.C., U.S. Environmental Protection Agency, Planning Assistance Branch).

Delaware River Ecologic Model

Kelley, R. A. 1975. "The Delaware Estuary Model," in C. S. Russell, ed., Ecological Modeling in a Resource Management Framework, RFF Working Paper QE1 (Washington, D.C., Resources for the Future).

ECOMOD

Water Resources Engineers, Inc. 1971. Effects of Waterfront Development on East San Francisco Bay, Report to Interagency Council on Waterfront Problems (Sacramento, Calif., Interagency Council on Waterfront Problems).

This report discusses the application of the Estuarine Ecologic Model (ECOMOD) to water quality conditions in East San Francisco Bay.

Yoder, Trotter, Orlob, and Associates. 1969. A Plan for a Comprehensive Water Quality Management Investigation, Report prepared for Association of Monterey Bay Area Governments (Santa Cruz, Calif., Association of Monterey Bay Area Governments).

This report presents the conceptual background for an estuarine ecologic model for use along the California Coast.

ECOFEM

Water Resources Engineers, Inc. 1975. Ecologic Modeling of Puget Sound and Adjacent Waters - Finite Element Ecologic Model: ECOFEM User's Manual, Report No. 6 (OWRT-C-2044-X)(Washington, D.C., U.S. Department of the Interior, Office of Water Resources Technology).

TRANS II

Resource Management Associates. 1976. Mathematical Simulation of Dynamic Density Stratified Flows in the Savannah Estuary, Report prepared for U.S. Army Corps of Engineers (Vicksburg, Miss., U.S. Army Corps of Engineers, Waterways Experiment Station).

ESTECO

Texas Water Development Board. 1977. ESTECO - Estuarine Aquatic Ecologic Model: Program Documentation and User's Manual (Austin, Texas, Texas Water Development Board).

This documentation report concentrates on the ecological relationships represented in ESTECO. The estuarine hydrodynamics associated with this model are provided by the two-dimensional HYD circulation model (see separate reference). Program listings are provided as well as program software components needed to apply this detailed ecologic model.

LAKE-1

Thomann, R. V., D. M. DiToro, R. P. Winfield, and D. J. O'Connor. 1976a. Mathematical Modeling of Phytoplankton in Lake Ontario: Part 1. Model Development and Verification, Report No. EPA-660/3-76-005 (Corvallis, Oregon, U.S. Environmental Protection Agency, National Environmental Research Center).

This report describes the mathematical modeling strategy for simulating phytoplankton dynamics in Lake Ontario. LAKE-1, a horizontally mixed lake with vertical layers, was calibrated and verified on available biological and chemical data. Preliminary development of a three-dimensional lake representation is also discussed.

__________, __________, __________, and __________. 1976b. Mathematical Modeling of Phytoplankton in Lake Ontario: Part 2. Simulations Using Lake 1 Model, Report No. EPA-600/3-76-065 (Duluth, Minn., U.S. Environmental Protection Agency, Environmental Research Laboratory).

This report describes the LAKE-1 simulation results of Lake Ontario for varying nutrient input levels. It illustrates the applicability of this model for traditional lake eutrophication problems.

Eutrophic Lake Quality Model

Baca, R. G. and R. C. Arnett. 1975. A Limnological Model for Eutrophic Lakes and Impoundments (Washington, D.C., U.S. Environmental Protection Agency, Office of Research and Development).

__________, __________, W. C. Weimer, L. V. Kimmel, H. E. McGuire, A. F. Gasperino, and A. Brandstetter. 1975. A Methodology for Assessing Eutrophication of Lakes and Impoundments (Washington, D.C., U.S. Environmental Protection Agency, Office of Research and Development).

CLEAN-CLEANER

Clesceri, L. S., R. A. Park, and J. A. Bloomfield. 1977. "General Model of Microbial Growth and Decomposition in Aquatic Ecosystems," Applied and Environmental Microbiology vol. 33, no. 5, pp. 1047-1058.

Haimes, R. and D. K. Leung. 1977. CLEANER Documentation - Version 3 (Troy, New York, Rensselaer Polytechnic Institute, Center for Ecological Modeling).

Scavia, D. and R. A. Park. 1976. "Documentation of Selected Constructs and Parameter Values in the Aquatic Model CLEANER," Ecological Modeling vol. 2, pp. 33-58.

WQRRS

Thorton, K. W. and A. S. Lessem. 1976. Sensitivity Analysis of the Water Quality for River-Reservoir Systems Model, Miscellaneous Paper Y-76-4 (Vicksburg, Miss., U.S. Army Corps of Engineers, Waterways Experiment Station).

This report evaluates the sensitivity of coefficients and initial conditions in the WQRRS model. A test program was developed to demonstrate the effects of changing one coefficient by 10 percent on 21 water quality variables. Overall model sensitivities were greater at high nutrient concentrations that at low concentrations. Other sensitive coefficients include evaporation and dispersion rates, biota growth, respiration, and temperature rates.

U.S. Army Corps of Engineers. 1975. Generalized Computer Program: Water Quality for River-Reservoir Systems, Computer Program Reports 401-F2-L2100 and 401-F2-L2100A (Davis, Calif., Hydrologic Engineering Center).

This documentation report describes the components of the Water Quality for River-Reservoir Systems Model. Because this model is continually upgraded by HEC, the user should attempt to obtain the latest version available.

__________. 1977. Water Quality for River-Reservoir Systems - Computer Program 401-F2-7100 (Davis, Calif., Hydrologic Engineering Center).

This computer documentation report represents the 1977 version of WQRRS documentation. It provides the most up-to-date user information for application to any riverine system or combination of river-lake systems.

Narragansett Bay Model

Hess, K. W. 1976. "A Three-Dimensional Numerical Model of the Estuary Circulation and Salinity in Narragansett Bay," Estuarine and Coastal Marine Science vol. 4, pp. 325-338.

This article discusses the basic formulations for a generalized, three-dimensional rigid lid model of steady, density-driven flow.

__________ and F. M. White. 1974. A Numerical Tidal Model of Narragansett Bay, Marine Technical Report 20 (Narragansett, R. I., University of Rhode Island).

This report describes the two-dimensional tidal hydrodynamic model used to represent Narragansett Bay circulation patterns. This model serves as the driving force for water quality-transport models developed later.

__________ and __________. 1976. Modeling the Dispersal of a Marked Fluid in Narragansett Bay, Marine Technical Report 38 (Narragansett, R. I., University of Rhode Island).

This report summarizes the application of a two-dimensional estuarine water quality model to trace the mass dispersal of a marked fluid throughout the Narragansett Bay system.

Spaulding, M. L. 1974. Laterally Integrated Numerical Water Quality Model for an Estuary, Marine Reprint 26 (Narragansett, R. I., University of Rhode Island, Sea Grant Program).

This brief article discusses the mass transport methodology used to simulate estuarine water quality.

__________, G. A. Brown, and F. M. White. 1974. Applying a Water Quality Model to Pollution Management, Marine Technical Report 26 (Narragansett, R. I., University of Rhode Island).

This article describes the use of a water quality model to simulate dissolved oxygen-BOD changes in Narragansett Bay under summertime conditions.

Chapter Five

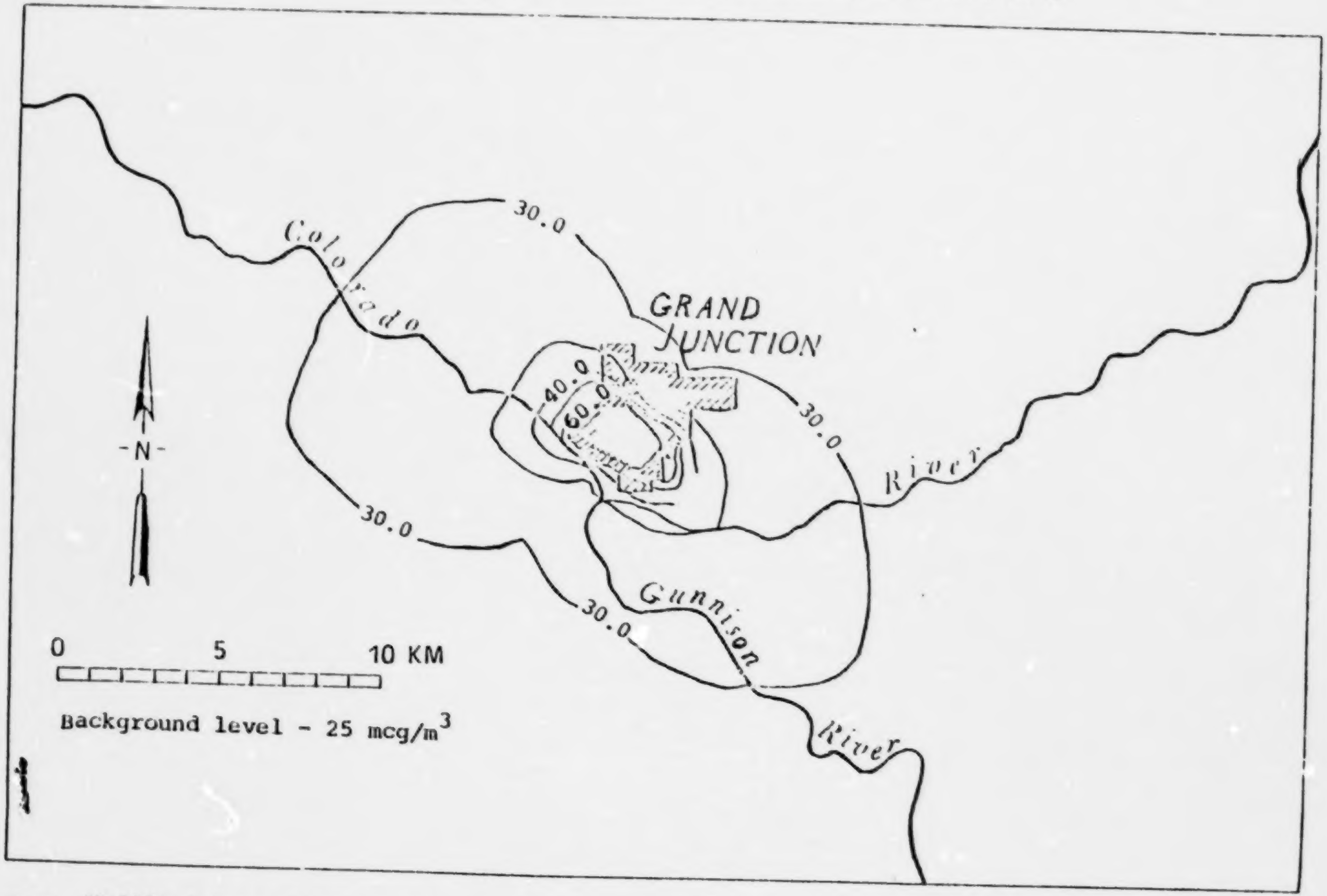
ANALYZING ATMOSPHERIC SYSTEMS

F. Douglas Muschett

INTRODUCTION

An atmospheric system is defined herein as a specified volume of air over a given land area. A typical atmospheric system extends vertically from the ground to the top of the atmospheric mixing layer, about 5 to 10 thousand feet in altitude, and horizontally encompasses regions on the order of 300 to 500 square miles. Horizontal boundaries of an atmospheric system are defined according to the areal extent of the land area of interest, e.g., metropolitan area defined by county boundaries, or the areal extent of a given air quality problem, e.g., usually defined as the area within a specified isopleth at a given point in time.[1] An isopleth is a line drawn on a map of a region connecting points of equal ambient concentration for a specified residual, as shown in figure 5-1. In figure 5-1, the atmospheric system in relation to the suspended particulate problem would roughly be defined by the volume enclosed by the 30.0 micrograms per cubic meter (mcg/m^3) isopleth. Beyond the 30.0 mcg/m^3 isopleth, the ambient concentrations of suspended particulates are generally 25.0 mcg/m^3 and are assumed to be primarily the result of natural sources, residuals entering the region from outside of the region, or both.[2]

Figure 5-1. Suspended Particulate Isopleth Map, Grand Junction, Colorado, 1970


Colorado River
GRAND JUNCTION
30.0
30.0
30.0
30.0
40.0
60.0
Gunnison River
-N-
0
5
10 KM
Background level - 25 mcg/m3

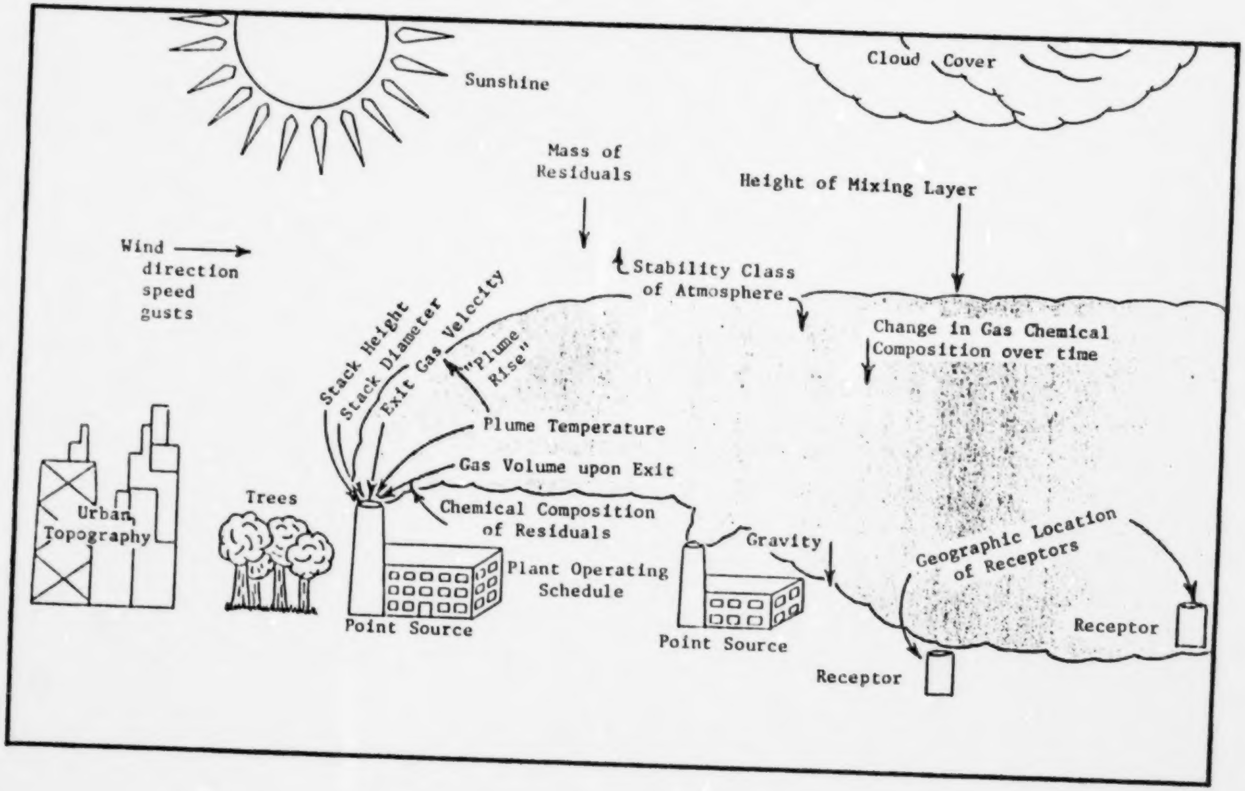
Source: Modified from Blair T. Bower, editor, Regional Residuals-Environmental Quality Management Modeling, RFF Research Paper R-7 (Washington, D.C., Resources for the Future, 1977).

Ambient air quality in an atmospheric system at any point in time is the result of both natural and man-made factors. Natural factors include sunlight, wind, precipitation, vegetation, topography including presence of water bodies, cloud cover, and temperature gradient. Man-made factors include: the spatial pattern and "topography" of structures; the types of activities, including agricultural operations and transport activities; the raw materials used in production; and the time patterns of gaseous residuals generation by and discharge from the activities. Some of the natural and man-made factors affecting ambient air quality are shown in figure 5-2. Various natural systems models (NSMs) have been developed which take more or fewer of these factors into account, in different degrees of detail. The purpose of this chapter is to provide background and information for selecting appropriate NSMs for analyzing atmospheric systems in various REQM contexts. NSMs used in analyzing atmospheric systems are generally referred to as air quality models.

The chapter is organized into four major sections. The first section briefly identifies some of the major ambient air quality problems associated with atmospheric systems, in relation to the combinations of meteorologic phenomena and residuals discharges which affect them. Only those combinations for which operational air quality models[3] have been developed are discussed. In addition, the section identifies and describes the key "operational" characteristics by which air quality problems can be described in relation to the NSMs developed to analyze them. Although this section is analogous to the first section in both chapter 3 and chapter 4, the discussion herein is considerably more brief than in those chapters.

The second section identifies and describes briefly the major atmospheric processes which affect the movement and transformation of residuals

Figure 5-2. Some Factors Affecting Ambient Air Quality


Sunshine
Cloud Cover
Mass of Residuals
Height of Mixing Layer
Wind direction speed gusts
Stability Class of Atmosphere
Change in Gas Chemical Composition over time
Stack Height
Stack Diameter
Exit Gas Velocity
"Plume Rise"
Plume Temperature
Gas Volume upon Exit
Chemical Composition of Residuals
Urban Topography
Trees
Plant Operating Schedule
Point Source
Gravity
Geographic Location of Receptors
Point Source
Receptor
Receptor

Source: N. F. Kron, and coauthors, Emission Density Zoning Guidebook, Publication No. EPA-450/3-78-048 (Research Triangle Park, N.C., Environmental Protection Agency, 1978) p. 14.

in atmospheric systems, movements and transformations which result in the air quality problems identified in the previous section. The extent and manner in which an air quality model includes the relevant atmospheric processes and the empirical data available to verify the model determine how accurately the model represents the real world.

The third section describes the basic approaches used to formulate air quality models. This section builds upon the related section in chapter 2, and explains how the general analytical approaches for analyzing natural systems are applied to atmospheric systems.

The fourth section indicates how to select, for any given REQM analysis context, one or more air quality models from a set of existing operational models. This section is directly related to the section in chapter 2 on setting up the analysis of natural systems. Four major elements comprise this section: (1) a listing of a large number of air quality models, both operational and nonoperational, referred to as the population table; (2) a table which relates air quality problem characteristics to the models listed in the population table, referred to as the problem table; (3) a flow diagram which indicates how to select an air quality model given the material in the chapter, referred to as the selection procedure; and (4) a discussion of the characteristics used to summarize the operational air quality models contained in Appendix A.

Appendix A contains detailed summary tables for 33 operational air quality models. Appendix B contains a list of annotated references for each of the models listed in the population table.

MAJOR PROBLEMS

Air quality models for analyzing air quality problems have evolved out of the need for quantitative information about the effects on man and on the environment resulting from the discharge of various material and energy residuals into the atmosphere. Once discharged into the atmosphere, residuals are transported or transformed, depending on existing meteorologic conditions and on the specified residuals discharged. The problems result from various spatial patterns of residuals concentrations prevailing over the earth's surface over time. In recent years, certain meteorologic conditions combined with discharges of residuals into the atmosphere have been identified as producing adverse impacts. The "problems" stemming from these combinations include: acid rain; transport of fugitive dust; pesticide volatilization and transport; transport of radioactivity; transport and deposition of toxic materials; transport and deposition of nutrients; transport of aeroallergens; formation and transport of sulfates; impacts on visibility; transport of "conventional" residuals such as sulphur dioxide (SO_2), total suspended particulates (TSP), carbon monoxide (CO), hydrocarbons (HC), and nitrogen dioxide (NO_2); and the formation and transportation of photochemical smog. Depending on the residuals discharged and the meteorologic conditions, residuals concentrations may cause adverse effects on humans, plants, animals, and/or inanimate objects, including various types of manufacturing and other productive processes.

Unfortunately, present knowledge of most of these problems is only rudimentary in terms of providing a basis for developing relevant operational air quality models. Hence, the scope of residuals discharge/meteorologic conditions combinations which can be analyzed using existing operational air quality models is limited. Of the problems identified above, operational models which existed in 1978 generally dealt only with combinations relating to the last two mentioned, the transport of conventional residuals and photochemical smog.[4] This section is, therefore, primarily limited to a discussion of problems relating to transport of conventional residuals and the formation and transport of photochemical smog.

Problems Relating to the Transport of Conventional Residuals

As indicated above, SO_2, TSP, CO, HC, and NO_2 are defined as conventional residuals. The term conventional is used for two reasons: (1) because there is some common agreement as to the negative impacts caused by high concentrations of these residuals in the atmosphere; and (2) because the majority of operational air quality models developed to date have dealt with analyzing the transport and transformation of these residuals. These five residuals along with photochemical oxidants are the "air pollutants" specified in the national primary and secondary ambient air quality standards for the United States.

Ambient concentrations of SO_2 and TSP are probably the two most widely used indicators of ambient air quality. Both are generated in the combustion of fossil fuels, e.g., coal and oil, and in various production processes. Particulates are also generated by a variety of other sources, e.g., wind erosion on agricultural lands, salt spray in coastal areas. Over the past three decades, increasing evidence has been generated on the adverse effects resulting from exposures to various duration-concentration combinations of these residuals.

First are the adverse effects on human health, both acute and chronic. Acute effects are those resulting from exposure to high concentrations of one or more residuals over a relatively short period of time, typically a few days. Chronic effects are those resulting from exposure over a long period of time, for example, as a result of living in an area with continuously poor ambient air quality.

Conditions of unusually high concentrations for a few days are referred to as episodic conditions. Although the primary mechanism through which human health is affected by poor air quality is inhalation, during episodic conditions other mechanisms are involved, such as those relating to nose and eye irritation. Acute health effects attributable to SO_2 and TSP relate primarily to the sudden aggravation of existing cardiorespiratory ailments in individuals during episodic conditions. Such conditions relating to SO_2 and TSP occur most often in winter months, when temperature inversions are more frequent, resulting in buildup of SO_2 and TSP concentrations over several days. Chronic health effects attributable to SO_2 and TSP relate to the high incidence of upper respiratory disease, pneumonia, and bronchitis in individuals residing primarily in urban areas. For further discussion of the health effects of SO_2 and TSP, see Suess and Craxford (1976) and Lave and Seskin (1977). Other adverse effects attributable to ambient concentrations of SO_2 and TSP include damage to plants (Davis and Wilhour, 1976) corrosion of building surfaces and machinery (SO_2), damage to paint films (SO_2), damage from deposition on building surfaces and materials (TSP), and physiological damage to fish and animals.

CO is primarily generated by the combustion of petroleum products, e.g., gasoline, in internal combustion engines in motor vehicles. CO is also generated in any activity in which carbonaceous fuels are incompletely combusted. Consequently, there is widespread exposure to CO, especially in urban areas.

Known adverse effects attributable to exposure to CO primarily relate to human health. Few or no adverse effects on plants and animals have been identified. When inhaled by humans, CO combines with elements in the blood (hemoglobin) and reduces the capacity of blood to carry oxygen from the lungs to other tissues. Inhalation of massive amounts of CO can cause death. Cases of such inhalation are very infrequent and only occur in small, improperly ventilated, interior spaces. With respect to ambient environmental quality, relevant adverse health effects relate to chronic exposure to low levels of ambient concentrations of CO. Most of the presently recognized adverse health effects relate to impacts on behavior and performance. For example, symptoms such as lassitude, headache, and impaired coordination have been observed. For additional information relating to the effects of CO on human health, see Committee on Effects of Atmospheric Contaminants (1969), Horvath, et al. (1971), Goldsmith and Landaw (1968), and chapters 7, 8, and 9 in U.S. Department of Health, Education, and Welfare (1970).

Both HC and NO_2 are precursors[5] to the formation of photochemical oxidants. This means that they react with other compounds in the atmosphere in the presence of sunlight to form oxidants. However, NO_2 also has adverse effects apart from those associated with photochemical oxidants. In contrast, ambient concentrations of HC have few recognized adverse effects independent from those caused by the oxidants produced in the photochemical oxidation process. For references to the relationship between hydrocarbons and human health, see Part II in U.S. Department of Health, Education, and Welfare (1970).

It is important to note that ambient concentrations of NO_2 and nitric acid (NO) have, historically, been added together and referred to as nitrogen oxides (NO_x). However, these two compounds have very different properties. NO is colorless and relatively nontoxic, whereas NO_2 is deep red-brown in color, toxic, and--as indicated above--is a precursor in the formation of photochemical oxidants. NO_2 is generated in the production processes in the chemical industries. NO is primarily generated in the combustion of fossil fuels, e.g., in motor vehicles and in power plants. In the ambient atmosphere, NO typically is converted to NO_2. The rate of this conversion depends on a number of factors, as discussed in Hazardous Materials Advisory Committee (1972).

Aside from impaired visibility, NO_2 in sufficiently high concentrations can irritate the eyes and throat, cause respiratory problems, and damage some dyes and fabrics. Epidemiologic evidence[6] indicates that NO_2 adversely affects lung function by decreasing the ventilative ability of the lungs, increasing the sensitivity of the lungs to other chemicals, and decreasing the defense mechanisms of the lungs. Some evidence exists that continuous exposure of certain plants to NO_2 causes severe defoliation and leaf chlorosis.[7] Although a number of studies have been performed to analyze the health effects of ambient NO_2, the evidence produced has been inconclusive and controversial. Present ambient standards apply only to annual average exposures to NO_2. However, in the 1977 Clean Air Act Amendments Congress required EPA to adopt a short-term standard for NO_2, unless EPA finds that such a standard is not needed to protect public health.[8]

Problems Relating to Photochemical Smog

Photochemical smog is the universally recognized term used to describe ambient air quality conditions associated with photochemical oxidants. The term "oxidants" refers to products formed in the atmosphere as the result of reactions between certain compounds, e.g., HC and NO_2, which reactions occur only in the direct presence of sunlight. Photochemical smog is therefore most frequent and severe during summer months. Photochemical smog is typically composed of oxidants such as ozone (O_3), PAN ($CH_3COO_2NO_2$), hydrogen peroxide (H_2O_2), formaldehyde (CH_2O), higher aldehydes (RCHO), acrolein (CH_2CHCHO), and formic acid (HCOOH). It is important to emphasize the distinction between this type of smog and the winter smogs produced from SO_2 and TSP discharges during temperature inversions.

The adverse effects of photochemical smog have been well documented over the past two decades. The literature contains an abundance of material on the subject, including comprehensive reviews in Organisation for Economic Cooperation and Development (1975) and National Research Council (1977).

Epidemiologic and controlled studies on humans and animals have provided a large body of information on human health effects of photochemical oxidants, although some disagreement still exists about the results of some of these studies. Presently recognized adverse health effects include decreased athletic performance, general discomfort, severe eye irritation, and increased respiratory problems.

Among the earliest recognized adverse impacts of photochemical oxidants were damages to vegetation. Early recognition was the result of very visible damage to leaf surfaces. Damages to vegetation and related microorganisms by oxidants is widespread among a large number of plant species. Adverse impacts range from chronic damage, i.e., decreases in annual crop yields per acre on agricultural and silvicultural lands, to acute damage, i.e., terminal effects.

It is important to indicate that, when one component of a natural system is affected, there usually are accompanying effects on other components of the natural system. Some of these "secondary" and "tertiary" effects may be more important than those on the component initially affected. For a detailed discussion of these interrelationships, see chapters 11 and 12 in National Research Council (1977). For a general discussion of ecosystem responses to changes in ambient environmental quality, see Appendix B to chapter 2.

Oxidants, principally ozone, also adversely affect materials, by such means as increasing their rates of deterioration. This is particularly true with respect to certain organic compounds such as natural rubber. Deterioration of synthetic rubbers, such as styrene, polypentadene, and polyisoprene, is also accelerated when they are exposed to low concentrations of ozone, on the order of 20-40 mcg/m^3, over time. Paint films are also damaged by ozone, reducing the life of such films. Some evidence also exists of adverse effects of ozone on textile products, especially cotton products.

Summary Comment on Major Problems

Two points merit mention concerning the analysis of air quality problems. First, the adverse effects identified above relating to the transport of conventional residuals and photochemical smog also relate to other combinations of residuals discharge/meteorologic conditions identified earlier.

Second, it is important to reemphasize that, even though national primary ambient standards have been set for these residuals to protect human health, considerable controversy remains as to: (1) whether the health effects indicated above can be attributed to any given airborne residual; and (2) what are acceptable ambient concentrations for a given residual. The relationship between human health and air quality is extraordinarily complex. It is very difficult to attribute mortality and morbidity to individual factors. For example, consider TSP concentration as an indicator of the hazard to public health of poor air quality. Only recently has sufficient scientific evidence been generated to stimulate reevaluation of this indicator by EPA (Council on Environmental Quality, 1978). The basis for this reevaluation is the recognition that in order to measure accurately the health impacts of particulates, the size distribution of the various particles which make up TSP must be determined.[9] Research has shown that only particles less than about 15 micrometers (microns) in size actually enter the respiratory tract. For additional discussion of this point, see Miller, et al. (1979).

Given the uncertainty surrounding the relative importance of various factors affecting ambient air quality and their impacts, it is nevertheless agreed that a strong association exists between the major problems mentioned above and poor air quality. It is also agreed that continued refinement is required of the quantitative tools for analyzing all aspects of air quality problems, including: models which estimate the discharge of residuals into the atmosphere; models which estimate the transport or transformation of residuals in the atmosphere, as discussed in this chapter; and models which estimate the impacts of various duration-concentration combinations of residuals on humans, plants, animals, and inanimate objects.

Key "Operational" Characteristics of Air Quality Problems

Regardless of the particular air quality problem, there are six key characteristics which can be used to describe operationally a given problem in relation to identifying air quality models which can be used for its analysis. They are: (1) type of residual; (2) type of source; (3) characteristics of receptor points; (4) type of terrain; (5) time properties; and (6) geographic scale. Depending on the specification of these characteristics, different air quality models would be applicable for a given problem in different contexts.

Type of residual is an important characteristic because different physical, physicochemical, and chemical processes must be considered in an air quality model depending on the residual or residuals of interest. It is important to emphasize that choices between or among NSMs would be made not only depending on which processes are included in a given model, but also on how well each process is quantitatively characterized.

Type of source relates to certain characteristics of the sources which discharge residuals of interest into the atmosphere. Source characteristics must be specified, because not all air quality models can analyze the effects on ambient air quality of all types of sources. Sources can be characterized as follows: (1) stationary point source, such as a factory, with one or many discharge points within the source, such as multiple stacks in the factory; (2) stationary area source involving either (a) an aggregate of individual discharge points, such as a neighborhood involving a number of individual residences which are not individually identified, or (b) an agricultural or silvicultural area from which particulates may be generated by wind or pesticides may volatilize from surfaces of plants and trees after spraying; and (3) line source which can be either (a) mobile, as a moving vehicle, or (b) stationary, as a dirt road which is subject to generation of particulates as a result of wind action. (Mobile sources are considered as area sources in some urban scale air quality models.) Sources can be further characterized with respect to the elevation of discharge, either as ground or elevated.

Receptor points are operationally defined as the points in a region at which estimates of ambient concentrations are desired. Important characteristics of receptor points are number, height, and spatial location. Receptor characteristics must be specified because air quality models vary with respect to their capabilities for producing estimates of concentrations at specified receptor locations.

Type of terrain is a particularly important problem characteristic. Most operational air quality models which have been developed to date are for smooth or gently rolling, open terrain, or for "rough" urban areas on smooth terrain.[10] Applying an air quality model to an area consisting of terrain features markedly different from those features for which the model was designed would produce meaningless estimates of concentrations. In some cases, the nature of the terrain may even preclude the use of an air quality model, especially a model based on the conservation of mass and energy approach.

Time properties of air quality models are usually defined as either long-term or short-term. Long-term and short-term are related to chronic and acute air quality problems, respectively, such as those relating to adverse health effects described above. The time period over which a concentration is estimated is termed the averaging period or averaging time. Long-term problems generally require air quality models capable of estimating annual average concentrations. Short-term problems generally require models that can estimate ambient concentrations for averaging periods on the order of 24 hours, 8 hours, 3 hours, or 1 hour. Air quality models which estimate ambient concentrations for such short averaging periods are often nonsteady state air quality models, because meteorologic and residuals discharge conditions are varied for each averaging period over the time period of the analysis and the estimates of concentrations for the previous period are inputs as initial conditions for the following period.[11] Models which estimate annual or seasonal average concentrations are usually steady state air quality models. In steady state air quality models the meteorologic and residuals discharge conditions can also be varied for each averaging period analyzed, e.g., year or season. However, estimates of concentrations from the previous period are not used as initial conditions for the following period.

It is important to note the large difference between the length of the averaging period and the number of successive averaging periods analyzed in a given analysis between air quality models used to analyze long-term problems and those used to analyze short-term problems. For example, short-term models are typically applied to problems relating to episodic conditions and, therefore, are run for an analysis period on the order of seven consecutive days. If a one hour averaging time were used, ambient concentrations would be estimated for 168 successive time periods. An annual average model would have to be run for 168 years to analyze a comparable number of time periods, a four-season average model for 42 years.

Geographic scale refers to the areal extent of the problem of concern. For application of current air quality models to problems, four geographic scales have been operationally defined: (1) up to a few kilometers (km); (2) from a few km to about 50 km; (3) from about 50 km to about 200 km; and (4) greater than 200 km. Models which analyze the transport of residuals on a scale of more than 200 km are called long-range transport models. No models of this type are described herein.

These problem characteristics are used later in the chapter--in the problem table--to identify the capabilities of specific air quality models.

MAJOR NATURAL PROCESSES

In any given atmospheric system, numerous natural processes are at work which transport and transform materials and energy. These processes, in conjunction with residuals discharges from man's activities and inputs of materials and energy from geocentric sources[12] result in the problems identified in the previous section. Materials which are not transformed during transport are termed nonreactive; those which are transformed during transport are termed reactive. (The terms nonreactive and reactive correspond to the terms conservative and nonconservative, respectively, used in chapters 2, 3, and 4.)

Three types of natural processes affect the transport and transformation of material and energy residuals in the atmosphere: physical processes; physicochemical processes; and chemical/photochemical processes. Biological and ecological processes have negligible effects on material and energy transport and transformation in atmospheric systems. Physical processes are also termed physical transport processes and include advection, diffusion (including turbulent wind fluctuations), and dry deposition. Physicochemical processes include rainout and washout. Chemical processes include chemical decay and photochemical oxidation.

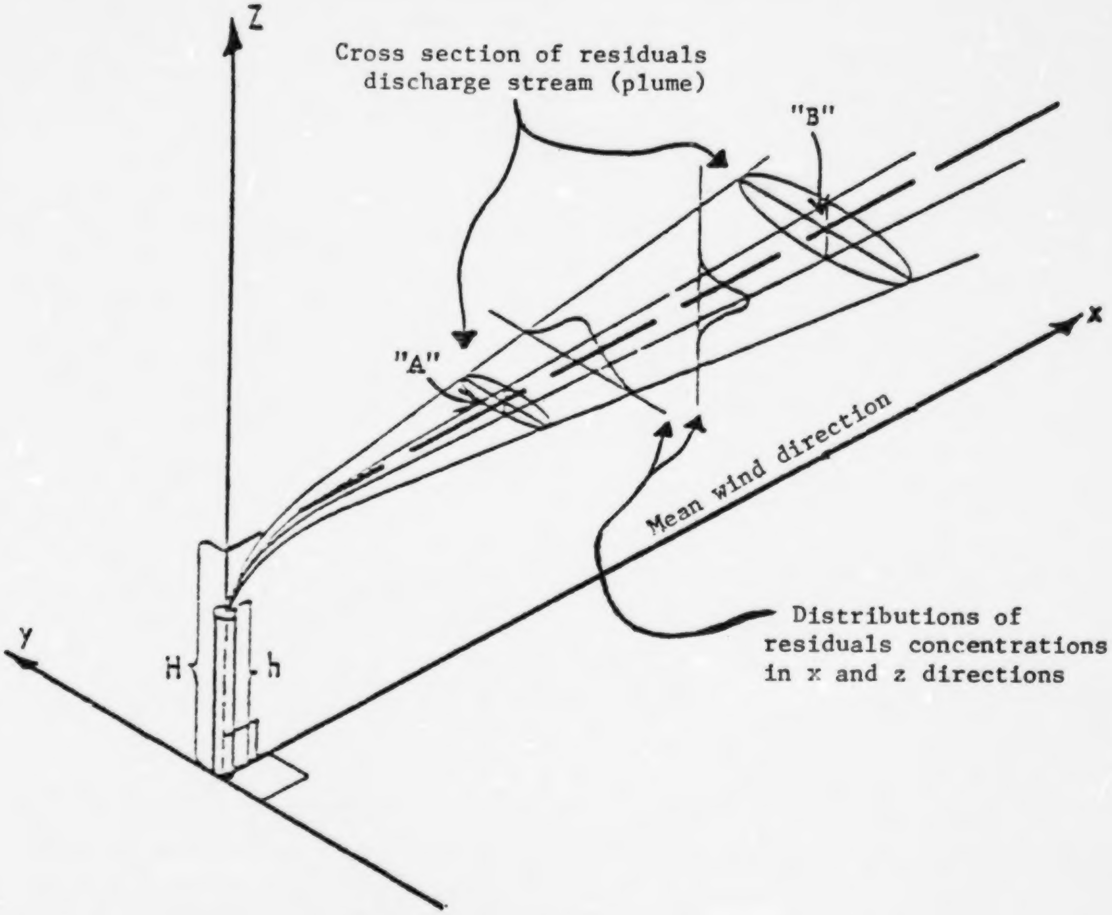
The extent to which NSMs of atmospheric systems consider these processes varies. Therefore, in order to select an appropriate NSM for a given REQM context, and to interpret the results after the NSM has been applied, it is important that the natural processes operating in atmospheric systems be understood.

Physical and Physicochemical Processes

Two basic physical processes account for the transport of material and energy in the atmosphere, advection and diffusion. Advection is the process by which materials and energy are transported through space by the movement of the medium within which they are suspended or dissolved. With respect to atmospheric systems this means that material or energy suspended or dissolved in air moves within an atmospheric system according to the air currents within that system, i.e., winds. Diffusion is a much more complicated transport process because several different kinds of diffusion may occur simultaneously in an atmospheric system. During the diffusion process, mass or energy within the air medium tends to move from regions of higher concentrations to regions of lower concentrations. Two important diffusion processes in atmospheric systems are thermal and mechanical turbulence. (Advection and diffusion are also defined in chapter 2.)

To illustrate the processes of advection and diffusion consider the discharge of gaseous residuals from a single stack, such as that shown in figure 5-3. Residuals discharged from the stack are more buoyant than the surrounding air and rise vertically to some height, H. As the residuals are rising to height H, they are being advectively transported by air currents in the mean wind direction. As the stream of residuals exiting the stack moves in the mean wind direction, the stream begins to "spread" due to diffusion. The spreading of the discharge stream is illustrated by the difference in the cross-sectional areas of the discharge stream at points A and B. Note that the cross section of the discharge stream is eliptically shaped. The discharge stream from a stack is commonly referred to as a "plume" because of its shape.

Figure 5-3. Illustration of Advection and Diffusion


Z
Cross section of residuals discharge stream (plume)
"B"
"A"
x
Mean wind direction
Distributions of residuals concentrations in x and z directions
y
H
h

Source: Modified from D. B. Turner, *Workbook of Atmospheric Dispersion Estimates*, Publich Health Service Publication No. 999-AP-26 (Cincinnati, Ohio, U.S. Department of Health, Education, and Welfare, 1969).

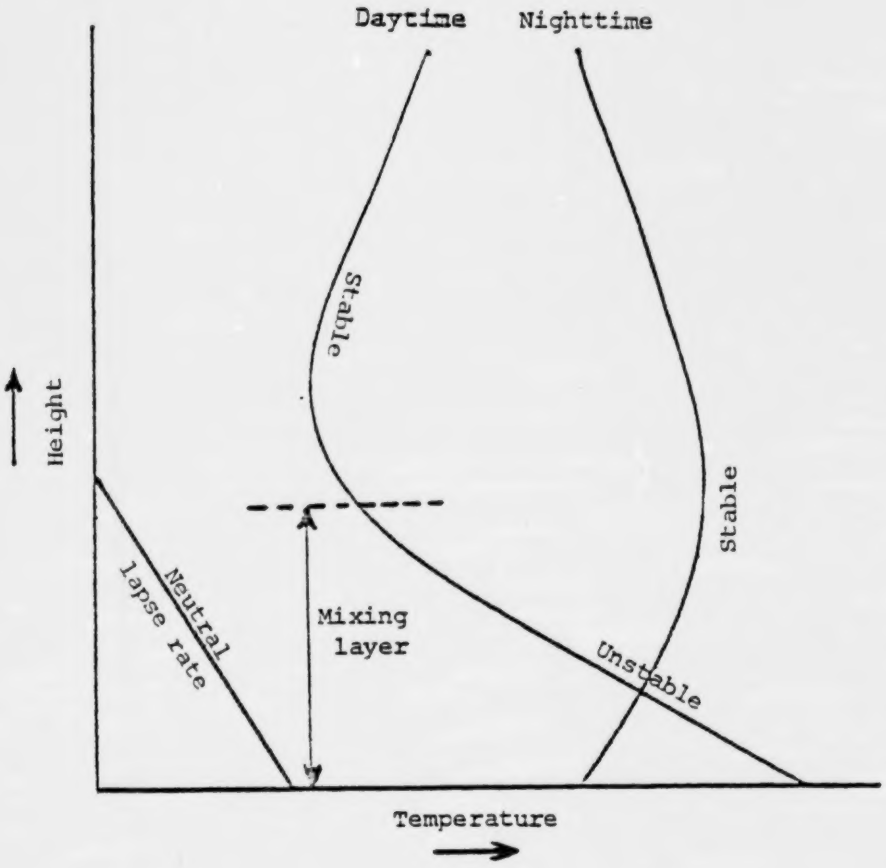
It is also important to note that the concentration of residuals within the plume is not uniform. Residuals concentrations are higher along the centerline of the plume than along the edges, as illustrated by the distributions of residuals concentrations in the y and z directions shown in figure 5-3. Also, at any point in time discharge plumes may be distorted in both the horizontal and vertical dimensions because of thermal and mechanical turbulent diffusion processes. The net effect of turbulent diffusion processes is highly variable ambient concentrations throughout the atmosphere over a given area.

Thermal turbulence is dependent upon the temperature profile of the atmosphere, that is, temperatures at different elevations above the ground at a given location. (This profile is sometimes referred to as the lapse rate.) During daytime the ground receives solar radiation, warms up and, in turn, warms the adjacent air. A temperature profile tends to develop in which temperature decreases quite rapidly with height for several hundred meters, as shown in figure 5-4. This profile promotes strong turbulent diffusion and stirring of the atmosphere in the vertical dimension; some of this turbulent energy is also transferred to the horizontal direction. This "unstable" atmospheric layer is referred to as the mixing layer.

During nighttime the reverse takes place. As the earth and adjacent air cool more rapidly than the layers of air farther away from the ground, a temperature profile develops in which temperature increases with height for several hundred meters above the ground. This situation is referred to as atmospheric inversion and results in relatively nonturbulent or stable conditions in the vertical dimension of an atmospheric system, as shown in figure 5-4.

Around sunrise and sunset an intermediate degree of thermal turbulence takes place. In this situation the temperature profile is in transition between stable and unstable conditions and is referred to as the neutral temperature profile or lapse rate. This situation is also shown in figure 5-4.

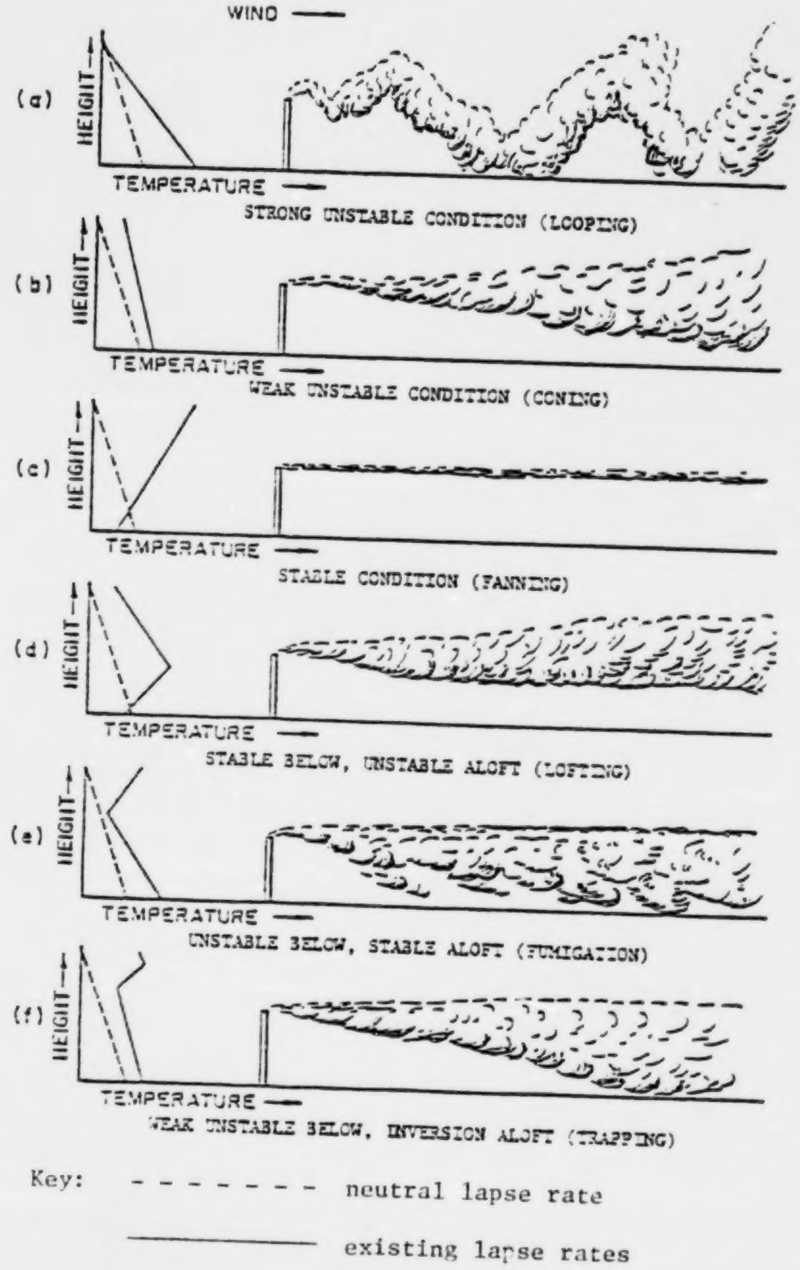
Figure 5-4. Vertical Temperature and Associated Stability Profiles


Daytime
Nighttime
Stable
Stable
Height
Neutral lapse rate
Mixing layer
Unstable
Temperature

The effects of thermal turbulence on discharge plume behavior are illustrated in figure 5-5. Of the six types of plume behavior shown, fumigation is very often the most important, because it causes very high, short-term ambient concentrations.

In the real world, the effects of thermal turbulence and diffusion are not as straightforward as described above, because many mitigating factors exist. Factors affecting thermal turbulence include: cloud cover; wind speed; and surface cover and topography, e.g., snow cover which reflects

Figure 5-5. Effects on Discharge Plume Behavior of Various Temperature Profiles

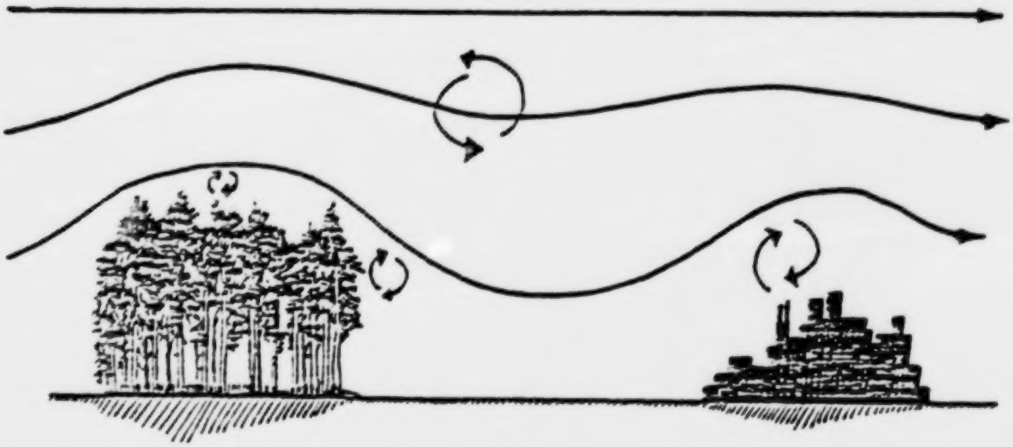

WIND
(a)
HEIGHT
TEMPERATURE
STRONG UNSTABLE CONDITION (LOOPING)
(b)
HEIGHT
TEMPERATURE
WEAK UNSTABLE CONDITION (CONING)
(c)
HEIGHT
TEMPERATURE
STABLE CONDITION (FANNING)
(d)
HEIGHT
TEMPERATURE
STABLE BELOW, UNSTABLE ALOFT (LOFTING)
(e)
HEIGHT
TEMPERATURE
UNSTABLE BELOW, STABLE ALOFT (FUMIGATION)
(f)
HEIGHT
TEMPERATURE
WEAK UNSTABLE BELOW, INVERSION ALOFT (TRAPPING)
Key:
neutral lapse rate
existing lapse rates

Source: E. W. Hewson, Industrial Air Pollution Meteorology (Ann Arbor, Michigan, University of Michigan, Department of Meteorology, 1960).

radiation and topography. For example, with respect to the last, snow cover reflects radiation particularly during the day, but causes unstable conditions at night; building structures in an urban area which absorb radiation during the day and release it at night have the opposite effect.[13] For additional discussion of thermal turbulence, see Hewson (1960) and Slade (1968).

Mechanical turbulence is caused by three factors: (1) frictional effects of the ground upon air flow; (2) terrain obstructions to air flow; and (3) vertical variations in wind speeds. Mechanical turbulence resulting from the movement of air along the ground surface is minimal in areas where terrain is flat and uniform and no hills or structures are interspersed over the surface, e.g., such as prairies or water bodies. However, when hills, mountains, heavy vegetation, or buildings are present, resulting mechanical turbulence can have a significant effect on the diffusion of a plume. Figure 5-6 illustrates this aspect of mechanical turbulence.

Figure 5-6. Mechanical Turbulence Caused by Uneven Terrain



Mechanical turbulence is indicated by circular flows.

Vertical variation in wind speed causes mechanical turbulence between layers of air traveling at different speeds, as the atmosphere tries to transfer momentum from layers of higher wind speeds to layers of lower wind speeds. The increase of wind speed with height generally causes a degree of mechanical turbulence throughout the mixing layer of an atmospheric system. For additional discussions of mechanical turbulence see Hewson (1960), Slade (1970), and Munn (1966).

The effect of thermal and mechanical turbulence on discharge plumes in terms of plume rise is especially important. Plume rise is defined as the vertical height above a discharge stack to which a discharge plume of residuals rises, as shown in figure 5-3, where plume rise = H - h. The final height of a discharge plume above the ground is equal to the stack height plus the plume rise. Plume rise is a function of the exit velocity and temperature of gases exiting a stack, the heat discharge rate from the stack, and meteorologic conditions, e.g., wind, air temperature, and turbulence. In most cases the heat discharge rate (buoyancy force) has more effect on plume rise than does the velocity of gases exiting the stack. Under these circumstances atmospheric stability is an important determinant of plume rise. When atmospheric conditions are stable and wind speed is light, plume buoyancy is reduced and the plume does not rise as high as under unstable conditions. When atmospheric conditions are unstable but wind speed is still light, plume buoyancy increases and the plume can rise very high. In some cases the plume can rise as high as 1000 meters, e.g., for very large sources such as power plants. When strong winds are present and atmospheric stability is neutral, plume rise will be negligible. For a detailed review of both qualitative and quantitative aspects of plume rise see Briggs (1969) and Briggs (1975).

Another important set of processes affecting residuals concentrations in the atmosphere consists of deposition processes. These result in transfers of material from the atmosphere to land surfaces and receiving water bodies. The two basic types of deposition processes are: dry deposition and wet deposition. Dry deposition is primarily a physical process, whereas wet deposition may be either a physical or physicochemical process. Dry deposition processes include gravity settling and impaction. Impact with a land or water surface usually occurs through turbulent mixing down to the land surface.

Wet deposition processes relate to the deposition of material from the atmosphere with falling water in the form of rain, fog, or snow. Two types of processes are involved: rainout and washout. The former involves the processes by which particles/substances are incorporated into water droplets within clouds; washout involves the processes by which particles/substances are attached to falling precipitation. The amount of material which is washed out or rained out of the atmosphere is a function of three factors: (1) the concentrations in the atmosphere of substances available for "scavenging;" (2) the effectiveness of precipitation in removing a given substance; and (3) the amount of precipitation. When suspended particles are washed out, the phenomenon is primarily a physical process. When substances are absorbed into hydrometeors,[14] either through in-cloud rainout and snowout, or through below cloud washout processes, the process is of a physicochemical nature. That is, the processes involve both the chemistry and physics of molecules as they interact in the atmosphere.

Significant adverse impacts on ambient environmental quality are produced by deposition of various residuals, such as lead, other heavy metals, pesticides, and nutrients (especially phosphorus but also nitrogenous compounds), on land surfaces and on water bodies. An increasingly recognized problem regarding deposition is the increasing acidification of precipitation, e.g., sulfuric acid, and nitric acid. In order to understand this phenomenon, knowledge is required not only of the deposition processes, but also of the chemical processes which transform residuals, such as SO_2 and NO_x, into acidic substances. Both the deposition processes and chemical transformation processes are not entirely understood at this time. Some of the chemical processes involved are discussed briefly in the next section.

It should be emphasized that deposition processes are not usually considered in air quality models designed to be applied to urban size areas, although they are often relevant, e.g., Mexico City, Chicago. Atmospheric deposition of residuals and its attendant effects on vegetation, aquatic systems, and soils, are generally considered to be interregional problems. Hence, these processes are considered only in long-range transport models. For additional information on atmospheric deposition see U.S. Forest Service (1976) and Robinson and Robbins (1971).

Chemical and Photochemical Processes

Chemical and photochemical processes involve the reaction of two or more compounds with each other to form one or more different compounds. Photochemical processes in the atmosphere are initiated by and dependent on the presence of sunlight, the amount and duration of irradiation determining the rates of the chemical reactions which take place. The number of reactions taking place in the atmosphere at any point in time is almost astronomical. Compounds are continually being created, destroyed, and recreated.

Regardless of the reaction, there are two basic types of chemical processes which take place, oxidation and reduction, and ionic dissociation. A chemical compound is oxidized when it loses one or more electrons to another compound. The compound receiving the electrons is said to be reduced. Ionic dissociation is the process whereby a compound separates (dissociates) into a simpler form without losing electrons.

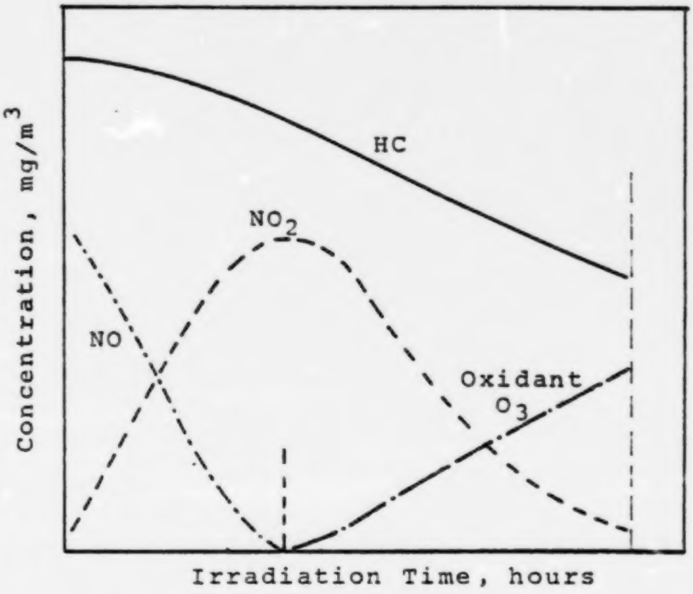
Among the myriad reactions that take place in the atmosphere, three types are of particular importance to air quality problems: (1) chemical decay reactions; (2) reactions leading to the formation of aerosols; and (3) photochemical oxidation. Chemical decay reactions relate to the chemical decomposition of gaseous residuals in the atmosphere. If strictly interpreted, this definition could cover all chemical reactions, because in every reaction one or more substances must "decay" to some extent. However, the terminology is used primarily in relation to reactions which reduce the concentration of a specified residual as it is transported over time from its origin of discharge. For example, if SO_2 is the residual of concern, the ambient concentration some distance downwind from a discharge source will be a function of wind speed, turbulence, plume rise, and the rate of decay of SO_2 in the atmosphere. It should be pointed out, however, that the amount of the residual which has decayed does not disappear, it is simply transformed into another form, a form which could be even more harmful than the original residual of concern. For example, the SO_2 which decayed in the above example is an input into the formation of other sulfur compounds, e.g., sulfates, including the formation of sulfuric acid in acid rain.

Aerosols traditionally have been defined as particles up to about ten microns in size which are suspended in the atmosphere. Because of their small size, aerosols remain in the atmosphere for extended periods of time, significantly longer than particulates of larger sizes. More than 80 percent of the mass of atmospheric aerosols is contained in the lowest kilometer of the atmosphere. Aerosols can be composed of any number of chemical compounds and enter the atmosphere from natural sources such as wind blown dust and soil, salt spray from the sea, smoke from forest fires, and from man-made sources. Aerosols are important with respect to the chemical processes operating in the atmosphere because they are also formed through chemical reactions among gaseous compounds and residuals in the atmosphere. (Such aerosols are termed secondary aerosols.) The most important aerosol formation reactions include: SO_2 reactions to form sulfate aerosols; NO and NO_2 oxidations to form nitrate aerosols; and hydrocarbon reactions to form organic aerosols. The presence of high concentrations of aerosols in the atmosphere affects many of the problems mentioned in the previous section.

Aerosol formation is particularly important in relation to deposition processes. Many of the harmful residuals which are deposited on land and water surfaces by these processes are aerosols which have been formed in the atmosphere and then scavenged out. An example is the formation of sulfuric acid in the atmosphere, which is essentially an aerosol formation reaction. For additional information about aerosols see chapter 3 in National Research Council (1977) and Robinson and Robbins (1971).

Photochemical oxidation is a chemical process whereby certain organic compounds in the atmosphere, e.g., hydrocarbons (HC) and nitrogen oxides (NO_x), are oxidized in the presence of light to produce oxidation products--oxidants--which are harmful. Figure 5-7 illustrates this process by showing the production of ozone--the major oxidant in photochemical smog--when NO, NO_2, and HC are irradiated in the atmosphere. The process shown in figure 5-7 is composed of two stages. First, NO is converted into NO_2. The second

Figure 5-7. Photochemical Production of Ozone



Source: Figure modified from Dimitriades, "Chemistry," in Assessing Transportation-Related Air Quality Impacts, Special Report No. 167 (Washington, D.C., Transportation Research Board, National Academy of Sciences, 1976) p. 9.

stage starts when all of the NO in the system has reacted. It is during this stage that ozone begins to form and accumulate until either the system uses up all of the available reactants or irradiation ceases.[15]

It is important to emphasize that the chemistry of photochemical oxidation is extraordinarily complex. For example, even if only one specific hydrocarbon compound were to be considered, and typical concentrations assumed for the other compounds required for photochemical oxidation of the hydrocarbon, several hundred chemical reactions would actually be involved in the oxidation processes (National Research Council, 1977). Recognizing that there are likely to be several hundred hydrocarbons in the atmosphere above an urban area--each with its own reaction rate and oxidation products--

underscores the complexity of photochemical oxidation reactions in the atmosphere.

The primary compounds responsible for the production of harmful oxidants in the atmosphere are nitrogen oxides and organics. The amount of oxidants produces in the atmosphere is dependent on time of day, meteorologic conditions, and the quantities of the primary compounds present. Time of day is important not only with respect to variation in meteorologic conditions, e.g., amount of sunlight, temperature, humidity, but also in relation to quantities of the primary compounds in the atmosphere. Because significant quantities of the primary compounds are discharged into the atmosphere from man's activities, oxidant production is very often related to the time pattern(s) of man's activities. This is especially true regarding the discharge of the primary compounds as residuals from vehicles. Residuals discharges from vehicles add large quantities of NO_x and hydrocarbons during morning and afternoon "rush hour" periods in urban areas. Oxidant formation in such areas tends to lag residuals discharges. Discharges of primary compounds from other sources tend to be more evenly distributed during the day.

For additional information on photochemical oxidation processes, see National Research Council (1977), and Organisation for Economic Cooperation and Development (1975).

APPROACHES TO ANALYZING ATMOSPHERIC SYSTEMS

This section describes briefly how the basic conservation of mass and energy and statistical approaches described in chapter 2 are applied to the analysis of atmospheric systems. It is important to emphasize that the material presented in this section is not a substitute for the detailed texts on the subject which are available. Rather, this section should be considered complementary to those texts, some of which are identified below.

Conservation of Mass and Energy Approach

Although the general principles of conservation of mass and energy are described in chapter 2, a few comments are nevertheless in order at this point. In all air quality models based on the conservation of mass and energy approach, the ambient concentration of a specified residual in a given volume of air is based on the mass of that residual entering and leaving the volume such that the total mass is accounted for, i.e., conserved. To illustrate this point, consider figure 5-8.

Figure 5-8 shows the three-dimensional sectioning of the atmospheric space above an urban area into unit volumes. Consider the sample unit volume extracted from the sectioned atmospheric space. Let I_1, I_2, and I_3 be the inputs of mass of a specified residual in relation to the three dimensions over some time interval of length Δt; let O_1, O_2, and O_3 be the outputs; and let T be the amount of mass transformed to some other form over Δt in the unit volume. Then:

$$\Delta M = I_1 + I_2 + I_3 - O_1 - O_2 - O_3 - T$$

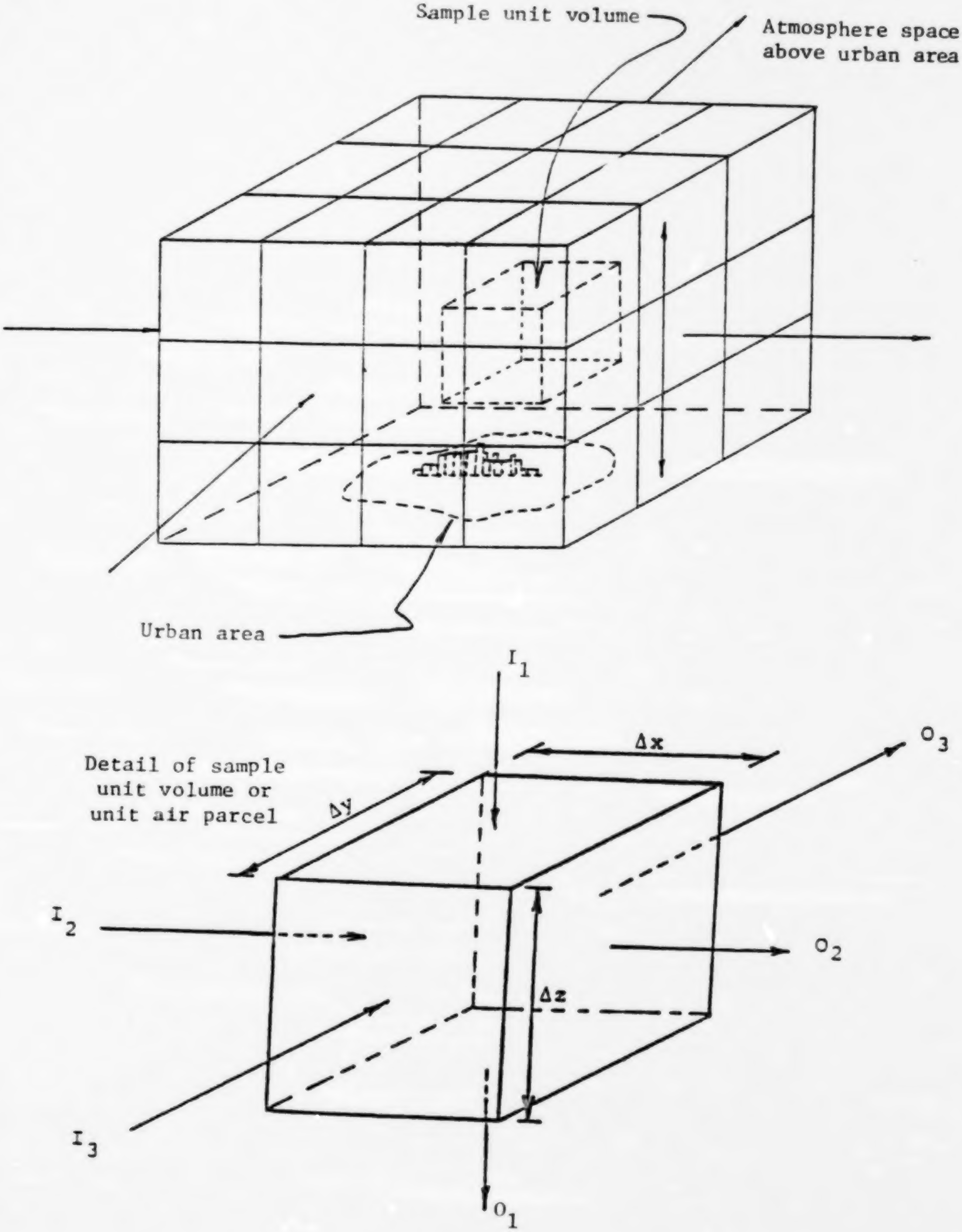
where ΔM is the change of mass in the unit volume during Δt, and

$$M_f = M_i + \Delta M$$

where M_f is the final amount of mass and M_i the initial amount in the volume.

The inputs, I_1, I_2, and I_3 consist of masses entering the volume due to the advection and diffusion of mass from adjacent unit volumes and from direct residuals discharges into the unit volume. Similarly, the outputs consist of masses leaving the volume due to advection and diffusion to adjacent unit volumes and by removal via "sinks" such as ground deposition.

Figure 5-8. Unit Volume Sectioning of Atmospheric Space to Illustrate Conservation of Mass and Energy Approach


Sample unit volume
Atmosphere space above urban area
Urban area
I_1
Δx
O_3
Detail of sample unit volume or unit air parcel
Δy
I_2
O_2
Δz
I_3
O_1

These relationships can be stated for the volume as follows:

$$\begin{array}{c}\text{Average rate of}\\\text{change of mass}\end{array} = \left(\begin{array}{c}\text{Average rate of inflow}\\\text{due to advection}\end{array}\right) - \left(\begin{array}{c}\text{Average rate of outflow}\\\text{due to advection}\end{array}\right)$$

$$[5\text{-}1] \qquad + \left(\begin{array}{c}\text{Average rate of inflow}\\\text{due to diffusion}\end{array}\right) - \left(\begin{array}{c}\text{Average rate of outflow}\\\text{due to diffusion}\end{array}\right)$$

$$\pm \left(\begin{array}{c}\text{Average rates from and}\\\text{to sources, sinks,}\\\text{and by reactions}\end{array}\right)$$

The standard three-dimensional differential form of equation [5-1], which is the basis for air quality models based on the principles of conservation of mass and energy, is:

[5-2]

$$\frac{\partial C}{\partial t} = \overbrace{- U_x \frac{\partial C}{\partial x} - U_y \frac{\partial C}{\partial y} - U_z \frac{\partial C}{\partial z}}^{\text{Advection}} + \overbrace{k_x \frac{\partial^2 C}{\partial x^2} + k_y \frac{\partial^2 C}{\partial y^2} + k_z \frac{\partial^2 C}{\partial z^2}}^{\text{Diffusion}} \pm S \pm R$$

where:

C = concentration (units/vol);

U_x = wind speed in x-direction (m/sec);

U_y = wind speed in y-direction (m/sec);

U_z = wind speed in z-direction (m/sec);

t = time (sec);

K_x, K_y, K_z = diffusivity coefficients for x, y, z directions, respectively (m/sec);

S = residuals discharge source or sink (units/sec/vol); and

R = reaction term (units/sec/vol).

Note that equation [5-2] is identical to the basic conservation of mass and energy equation stated for receiving water bodies in chapter 4.

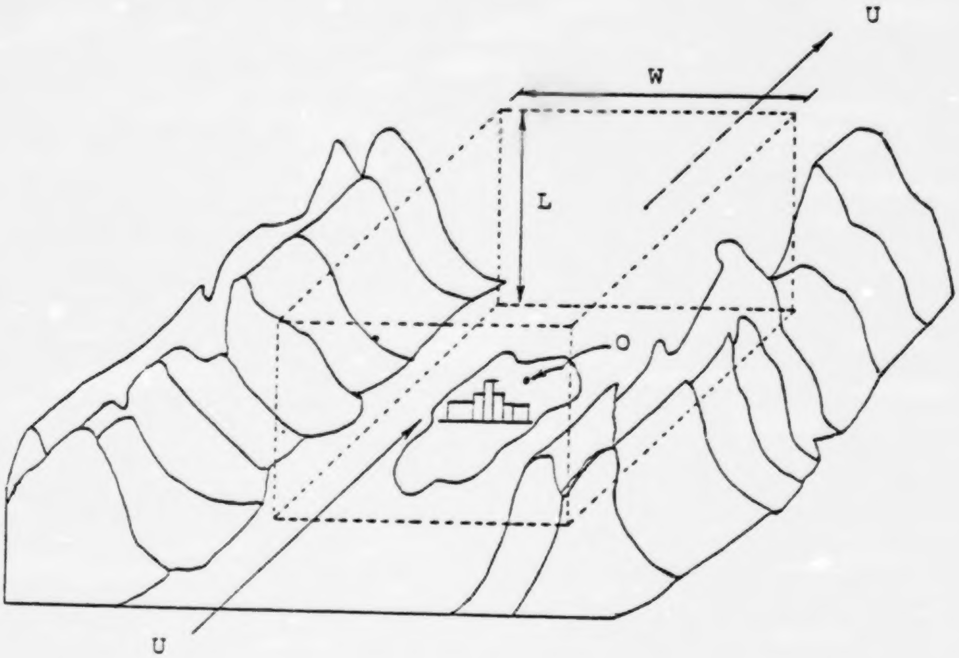
Air quality models based on the principles of conservation of mass and energy can be operationally separated into three categories of analytical approaches: volumetric, Gaussian, and numerically integrated.

The distinction among these categories is degree of complexity, which reflects the extent to which each approach explains the actual phenomena operating in the atmosphere. The volumetric approach is by far the simplest and treats the atmospheric space above an area of interest as a single homogeneous volume. The Gaussian approach--in its various forms--is more complex and is based on analytical integrations of equation [5-2] under certain simplifying assumptions. The numerically integrated approach is the most complex and, as the term implies, is based on numerical integration of equation [5-2]. Photochemical reactive models represent an important subcategory of the numerically integrated approach. These models involve numerical integration of equation [5-2], but also include sets of equations--in relation to the R term in the equation--which take into account photochemical oxidation processes and yield estimates of ambient oxidant concentrations. The remainder of this section discusses these three approaches.

Volumetric Approach

Models which are based on this approach are typically referred to as "box models." This is because the atmospheric space to some height above an area of interest is considered to be one large volume, i.e., as if a box were placed over the area, as depicted in figure 5-9. This approach assumes: (1) that there is instantaneous mixing of residuals discharged within the box into a volume of air entering the upwind side of the box during time period t; and (2) that steady state conditions exist in which the mass of residuals leaving the box through the downwind side is equal to the mass entering the box due to residuals discharges. Thus, mass is assumed to enter the box only due to residuals discharges within the box and all residuals discharged into the box exit the box. For point O in figure 5-9,

Figure 5-9. Volumetric "Box Model" for City in a Valley



the ambient concentration of a specified residual can be computed using the following formula:

$$C = \frac{Q}{ULW}$$

where C = concentration (units/m^3);

Q = upwind residuals discharge into box (units/sec);

U = wind speed (m/sec);

L = mixing height (m); and

W = valley width (m).

Most models caution that models based on the volumetric approach should be used only for first cut approximations because of the severe assumptions involved in the approach. For example, the assumption that residuals discharges are instantaneously mixed in the volume upwind from a receptor point tends to underestimate concentrations at the receptor point. On the other hand, if all residuals discharges into the volume are considered, instead of only discharges upwind from a specified receptor point, then the concentrations at the receptor point tend to be overestimated. However, in circumstances in which conditions closely match the conditions assumed by the approach, reasonable estimates of concentrations can be made, such as estimating short term concentrations--up to a few hours--for an urban area in a valley during a time period in which both the mixing height and residuals discharges remain fairly constant. Briggs (1973) suggests that the volumetric model could also be used to estimate concentrations downwind of a large single source during the early morning "fumigation" period when elevated plumes are rapidly mixed to the ground, as solar heating of the ground builds a turbulent layer up to and above the plume height.

Gaussian Approach

The Gaussian approach is based on analytical integration of equation [5-2], which assumes that the concentration of a residual in the discharge plume downwind from a source is normally distributed in each dimension. This assumption can be illustrated by referring to figure 5-3, which shows a discharge plume with normal or Gaussian distributions of residuals concentration in two dimensions. Many variations of the Gaussian approach have been developed. In addition to the assumption of Gaussian distributions of residuals concentrations, each variation is based on a different set of simplifying assumptions. The three most important Gaussian formulations are: the instantaneous "puff" formula, the continuous plume formula, and the line source formula. Short discussion of these formulae follow.

The instantaneous "puff" formula is analogous to the Gaussian formula presented in chapter 4 for estimating downstream concentrations due to an instantaneous discharge of a "slug" of conservative material into a river. Figure 5-10 illustrates what is meant by an instantaneous puff discharge and shows the Gaussian distributions assumed for residuals concentrations within the puff. In order to integrate equation [5-2] analytically, certain "boundary conditions" must be designated and certain assumptions made. In addition to the assumption of Gaussian distributions of concentrations in each of the three dimensions, the following three assumptions are required:

1. the average wind is defined as being in the x-direction, i.e., $U_y = 0$;
2. vertical transport is neglected, i.e., $U_z = 0$; and
3. spatially homogeneous turbulent diffusion processes are present.

Analytically integrating equation [5-2], based on the above assumptions, produces the generic equation on which all Gaussian puff models are based, that is:

$$[5\text{-}3] \qquad C = \frac{Qe^{-\left[\frac{(x-Ut)^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{z^2}{2\sigma_z^2}\right]}}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}$$

where:

C = concentration (units/m^3);

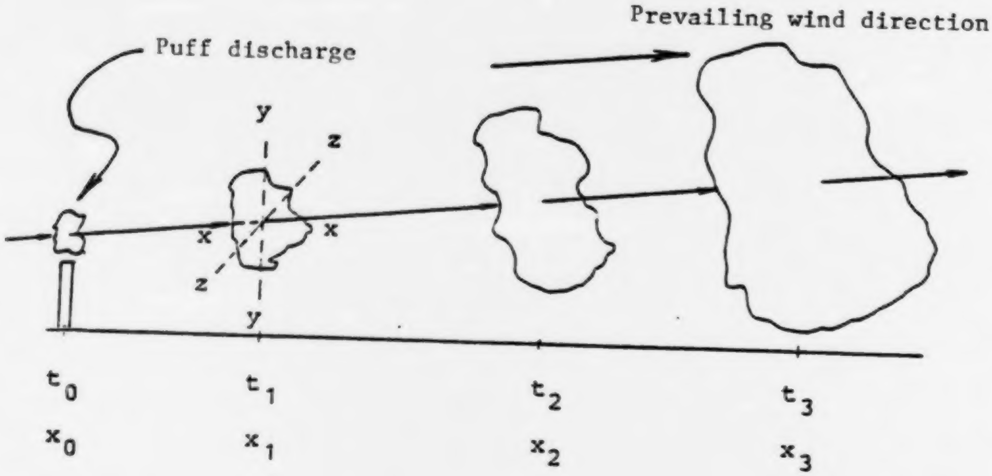
Q = total mass discharged (kilograms);

σ_x = $2k_xt$, puff diffusion in x-direction (m);

σ_y = $2k_yt$, puff diffusion in y-direction (m);

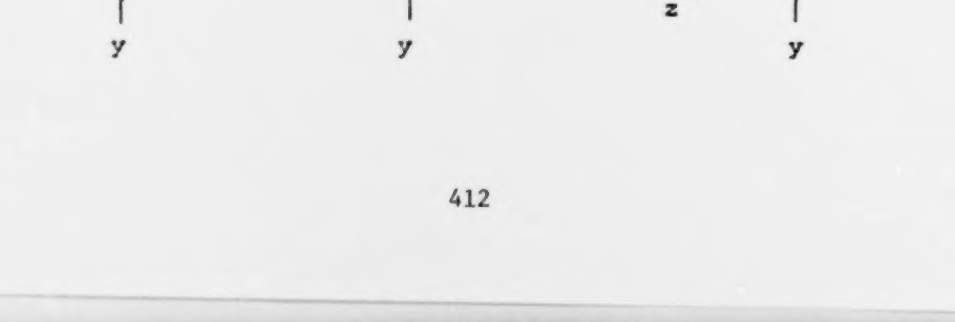
σ_z = $2k_zt$, puff diffusion in z-direction (m);

Figure 5-10. Illustration of Instantaneous Puff Discharge and Gaussian Distribution Assumption


Prevailing wind direction
Puff discharge
y
z
x
x
z
y
t_0
x_0
t_1
x_1
t_2
x_2
t_3
x_3

t = time; x = distance

Assumed Gaussian distributions of residuals concentrations in each dimension of puff at downwind distance x_1:


y
x
x
y
y
x
x
y
y
z
z
y

K_x, K_y, K_z = diffusivity coefficients for x, y, and z directions, respectively (m/sec);

U = mean wind speed (m/sec);

x = downwind distance at which C is to be estimated (m); and

t = travel time of puff (sec).

σ_x, σ_y, and σ_z represent the standard deviations of the concentration distributions in the puff, and are used so that equation [5-3] can be expressed directly in terms of the dimensions of the puff. A number of Gaussian puff models are summarized in Appendix A.

The continuous plume formula was developed to estimate downwind concentrations from a source with a continuous rate of discharge. Figure 5-3 illustrated what is meant by a continuous plume. In addition to the Gaussian assumption regarding plume spread, the following assumptions are required:

1. the rate of discharge from the source is uniform and continuous;
2. the mean wind speed affecting the plume is in the x-direction;
3. the plume is totally reflected at the earth's surface, i.e., no deposition on or reaction with the surface takes place;
4. diffusion in the x-direction can be neglected; and
5. steady state conditions prevail.

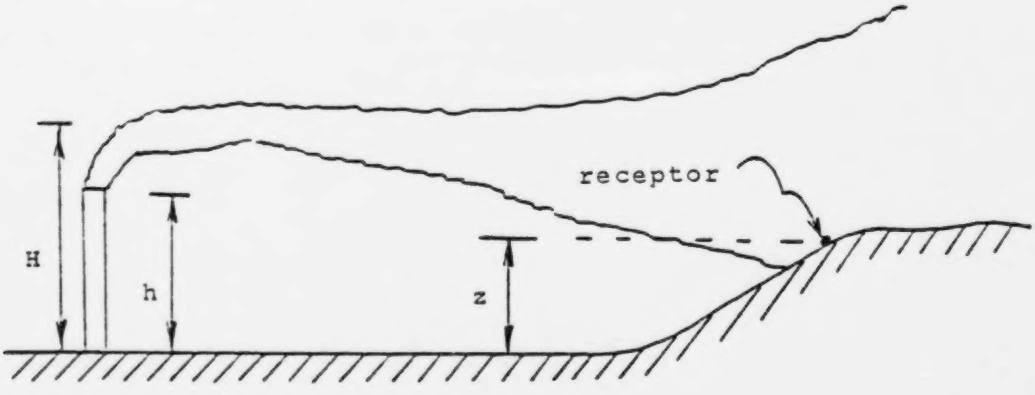
Turner (1969) indicated that diffusion in the x-direction can be neglected if the discharge is continuous or if the duration of the discharge is equal to or greater than the time of travel from the source to a location of interest. Analytical integration of equation [5-2] based on these assumptions produces the following short-term Gaussian equation:

[5-4] $$C = \frac{Q}{2\pi\sigma_y\sigma_z U}\left[e^{-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2}\right]\left[e^{-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2} + e^{-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2}\right]$$

where:
C = concentration (units/m^3);
Q = discharge rate (units/sec);
H = effective stack height (m);
σ_y = $2K_y t$, horizontal plume diffusion parameter (m);
σ_z = $2K_z t$, vertical plume diffusion parameter (m);
U = wind speed (m/sec);
z = receptor height (m); and
y = receptor crosswind distance from plume (m).

Figure 5-11, below, shows the relationship among stack height, effective stack height, and receptor height.

Figure 5-11. Relationship among Stack Height, Effective Stack Height, and Receptor Height



H = effective stack height
h = stack height
z = receptor height
H - h = plume rise

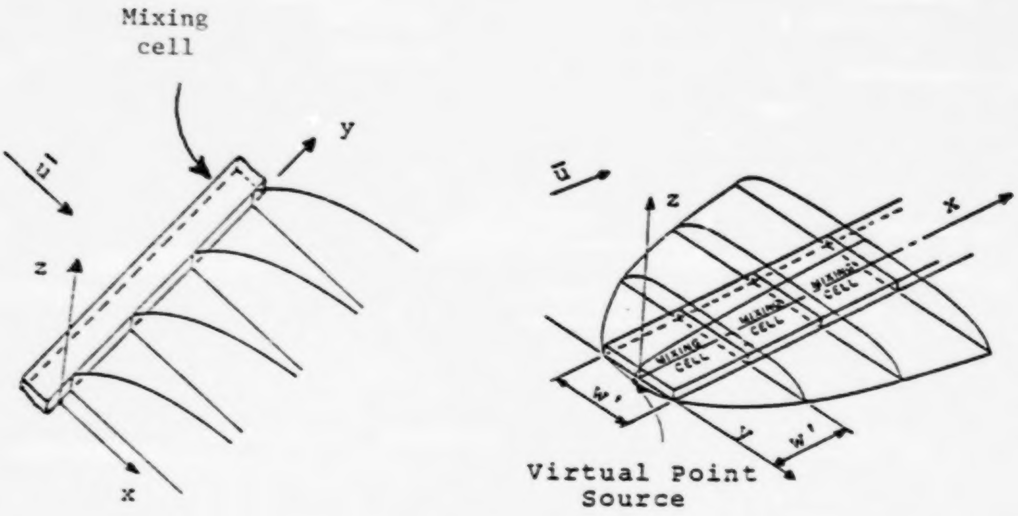
For many applications equation [5-4] is simplified. For example, if concentrations were to be calculated only at ground level, z would equal zero, and the terms $e^{-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2}$ and $e^{-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2}$ would become $e^{-\frac{1}{2}\left(\frac{-H}{\sigma z}\right)^2}$ and $e^{-\frac{1}{2}\left(\frac{H}{\sigma z}\right)^2}$, respectively. If the discharge were at ground level and there were no plume rise, effective stack height, H, would also go to zero and the equation would be further simplified. Turner (1969) provides additional information with respect to the conditions under which the continuous plume formula can be simplified.

The line source formula is based on equation [5-4] and is also referred to as the continuous "infinite" line source formula. The line source formula has been used primarily in relation to estimating the dispersion of gaseous residuals discharges from automobiles traveling along roads and highways. Important to the use of the line source formula is the mixing cell concept. A mixing cell is defined to be a well-mixed region surrounding a highway which would not be affected by surface atmospheric stability. The mixing cell is used as a uniform well-mixed discharge source from which residuals are dispersed downwind in a Gaussian manner (Ward and Ranzieri, 1976). Figure 5-12 illustrates the dispersion of gaseous residuals from a line source represented as a mixing cell.

The general line source Gaussian formula is derived by analytically integrating equation [5-4] in the y-direction. The resulting equation pertains to dispersion conditions in which the mean wind direction is crosswind to the line source, as shown in figure 5-12A. The resulting line source equation is:

$$[5\text{-}5] \qquad C = \frac{Q}{\sqrt{2\pi\sigma_z U}}\left[e^{-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2} + e^{-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2}\right]$$

Figure 5-12. Illustration of Dispersion of Residuals Discharges from an Infinite Line Source Represented as Mixing Cell



5-12A. Dispersion due to crosswinds

5-12B. Dispersion due to parallel winds

$\bar{u}$ = mean wind direction

w' = width of mixing cell

Source: Modified from C. E. Ward, Jr., and A. J. Ranzieri, "ÇALINE 2: An Improved Microscale Model for the Diffusion of Air Pollutants from a Line Source," in Transportation Research Board, Assessing Transportation-Related Air Quality Impacts, Special Report No. 167 (Washington, D.C., Transportation Research Board of the National Academy of Sciences, 1976) figures 10 and 12, p. 107.

where H is the height of the road above the land surface and all other variables are as defined for equation [5-4]. In order to use equation [5-5] in conjunction with the mixing cell concept of line source discharge, a number of assumptions are required. Ward and Ranzieri (1976) identify the set of assumptions listed below. They are instructive in terms of the limitations on the use of the formula.

Summary of Assumptions

1. Gaussian (normal) dispersion of residuals occurs in horizontal and vertical directions of plane perpendicular to wind direction.

2. A uniform wind flow field exists, with no vertical wind shear or aerodynamic eddies from uneven surface roughness.

3. No buildup of inert pollutants occurs due to elevated inversion conditions for microscale estimation of concentrations.

4. No chemical reactions or gravitational settling occur that affect the residual during the period of analysis.

5. Vehicles using the line source represent a continuous and constant source of discharges.

6. The initial vertical dispersion of residuals within the mixing cell is twice the height of the average vehicle (or 4 m) and the initial horizontal dispersion is a function of the highway width.

7. Residuals are uniformly distributed throughout the mixing cell region regardless of surface atmospheric stability conditions.

8. Perfect plume reflection occurs when the plume intersects the ground surface.

9. Parallel winds cause a buildup of residuals.

10. A line source having a width W can be approximated by a series of square area sources with W-length sides, which can in turn be approximated by virtual point sources.

11. A finite highway segment can be approximated by "infinite" line source equations.

12. Pasquill stability classes and modified dispersion parameters adequately describe the turbulence of the atmosphere.

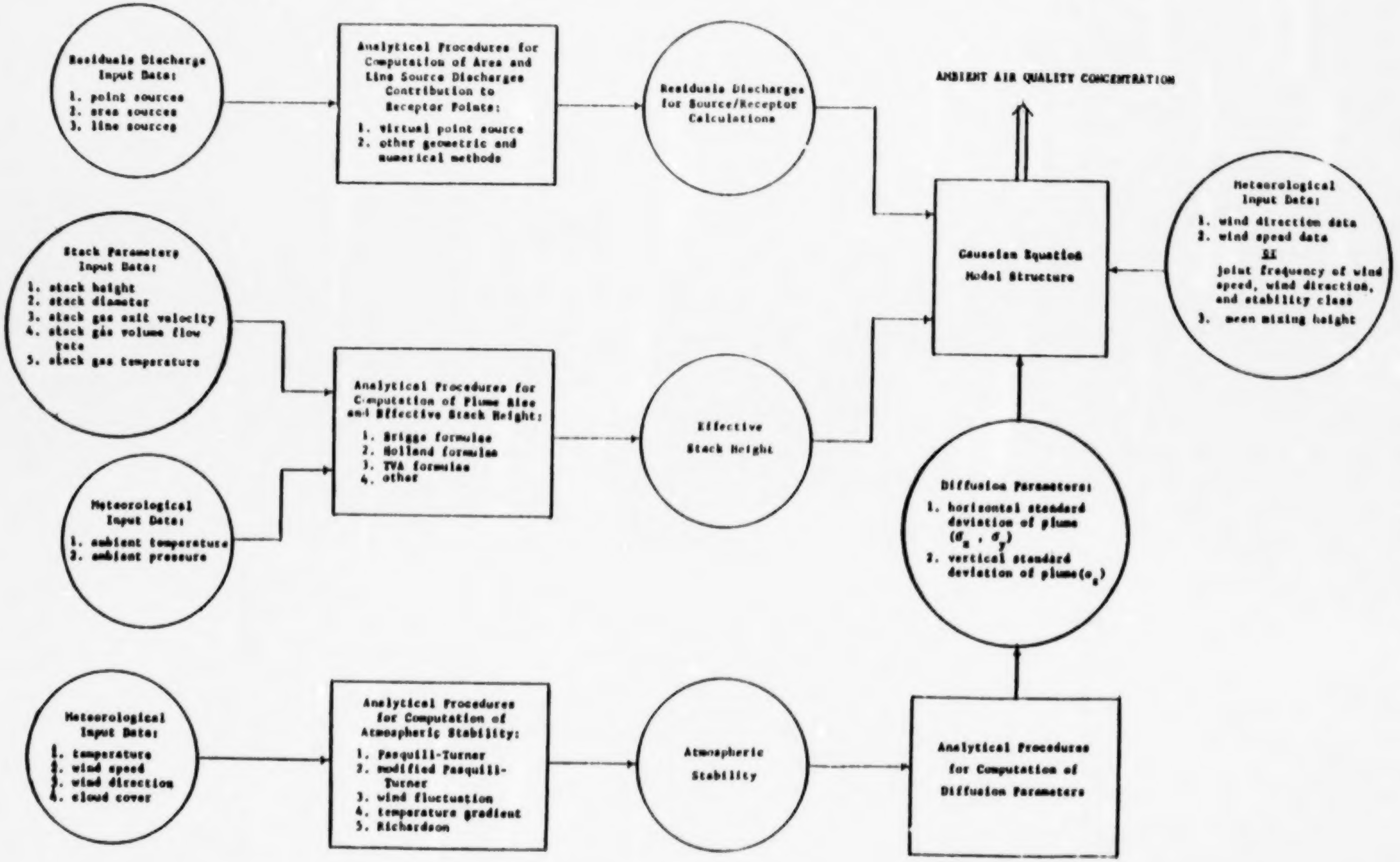
13. Only estimates of concentrations above ambient levels are made.

In cases where prevailing winds are parallel to the line source, as is depicted in figure 5-12B, equation [5-4] can be applied directly by using the virtual point source method to characterize residuals discharges from area sources. The mixing cell would be treated as a series of small area sources, each having the same quantity of residuals discharges but at different distances from a specified receptor. (The virtual point source method is discussed briefly in the discussion which follows.) Any number of virtual point sources could be used to represent the line source; the downwind concentrations from each would be summed together to estimate the total ambient concentration at a specified location.

Regardless of the specific model, the application of all Gaussian air quality models involves certain components, i.e., data and analytical procedures to process the data into the requisite variables whether they are explicitly incorporated into the model or not. Figure 5-13 identifies these components and illustrates how they form inputs into the Gaussian model structure. It should be emphasized that a given operational model does not normally contain all of the individual data inputs shown on the figure, nor does it require all of the analytical procedures shown. For example, with respect to the computation of plume rise, one model may use the Briggs formulae while another uses the Holland formulae. The figure is only meant to be illustrative of the types of data inputs required and the analytical procedures necessary to implement a typical Gaussian model. The components are briefly discussed below.

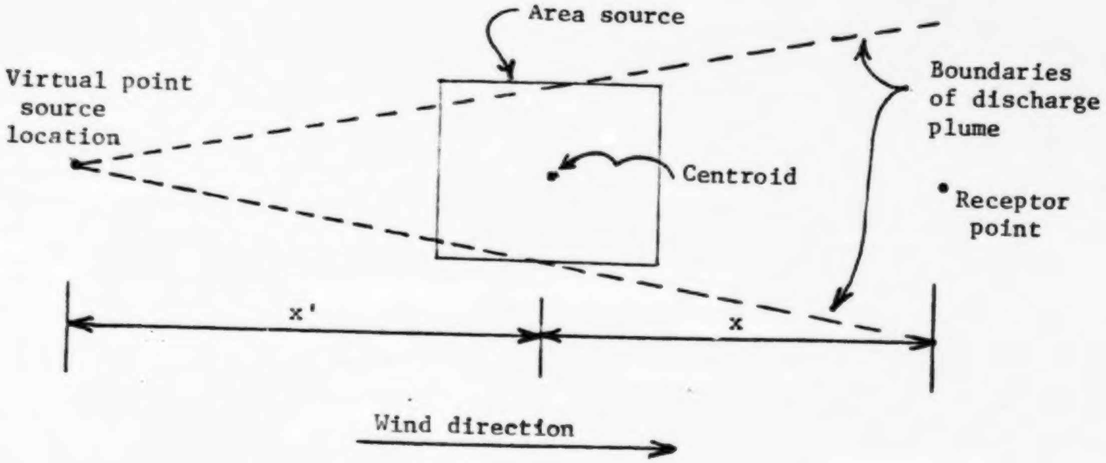
All Gaussian models require residuals discharge inputs. Depending on the problem contexts, these data may be input as discharges from point sources, area sources, line sources, or all three. Models which only consider a limited number of point sources and concentrations at a limited number of point receptors are straightforward. As indicated above, concentrations from the respective point sources are summed at a given receptor point. When the effect of an area source upon a receptor point is considered, for a given set of meteorologic conditions, some models utilize the "virtual point source" approach.

Figure 5-13. Schematic of Gaussian Model Components: Data Inputs and Analytical Procedures.


Residuals Discharge Input Data:
1. point sources
2. area sources
3. line sources
Analytical Procedures for Computation of Area and Line Source Discharges Contribution to Receptor Points:
1. virtual point source
2. other geometric and numerical methods
Residuals Discharges for Source/Receptor Calculations
AMBIENT AIR QUALITY CONCENTRATION
Gaussian Equation Model Structure
Meteorological Input Data:
1. wind direction data
2. wind speed data
OR
joint frequency of wind speed, wind direction, and stability class
3. mean mixing height
Stack Parameters Input Data:
1. stack height
2. stack diameter
3. stack gas exit velocity
4. stack gas volume flow rate
5. stack gas temperature
Meteorological Input Data:
1. ambient temperature
2. ambient pressure
Analytical Procedures for Computation of Plume Rise and Effective Stack Height:
1. Briggs formulae
2. Holland formulae
3. TVA formulae
4. other
Effective Stack Height
Diffusion Parameters:
1. horizontal standard deviation of plume (σ_x , σ_y)
2. vertical standard deviation of plume(σ_z)
Meteorological Input Data:
1. temperature
2. wind speed
3. wind direction
4. cloud cover
Analytical Procedures for Computation of Atmospheric Stability:
1. Pasquill-Turner
2. modified Pasquill-Turner
3. wind fluctuation
4. temperature gradient
5. Richardson
Atmospheric Stability
Analytical Procedures for Computation of Diffusion Parameters

Not all specified data inputs and analytical procedures are required with a given operational model.

Figure 5-14. Representation of Virtual Point Source Approach


Area source
Virtual point source location
Boundaries of discharge plume
Centroid
Receptor point
x'
x
Wind direction

The virtual point source approach is an analytical procedure whereby an area source may be translated into a roughly equivalent point source, so that a Gaussian point source formula can be applied. The procedure is shown in figure 5-14, above. By considering an area source as a virtual point source, a distance x' can be determined such that the plume width from a point discharge a distance of x' upwind from the centroid of the area source would be equal to the width of the area by the time the point source discharge reached the centroid of the area. A point source Gaussian formula could then be applied to the virtual point discharge at a distance x' + x from the receptor location to simulate the downwind effect of the area source.

Although the virtual point source procedure is simple and effective, it is very tedious in contexts where there are many area sources and receptor locations, because the procedure must be applied for each area source-receptor location combination. However, more efficient procedures have been developed to enable more efficient analysis of area sources, as discussed in references for the Climatological Dispersion Model in Appendix B.

Depending on the context, other analytical procedures may also be required to compute concentration contributions from area and line source discharges. For example, when a recpetor location is close to an area source, or within an area source, the source/receptor geometry is very important for determining the contribution of the source to the ambient concentration; the same is true for line sources. For additional information on analytical procedures for such cases see references for Point, Area, Line Source Model in Appendix B.

Stack parameters such as stack height, stack diameter, and stack exit gas velocity, volume, temperature, and meteorologic data such as ambient temperature and pressure, are important inputs for determining plume rise and effective stack height. These data may be input into a number of standard formulae in order to estimate the plume rise for a given point source. Most operational models use the Briggs (1969 and 1975), Montgomery (1974), or Holland formulae. Each formula is composed of individual formulae for specific atmospheric stability conditions.

The Briggs formulae were originally developed from theoretical principles, with subsequent observational testing, whereas the Holland and TVA formulae are empirically based. The TVA formulae are primarily applicable to large power plant sources, while the other formulae are more general. The Holland formulae are widely recognized systematically to underestimate plume rise for large, buoyant sources and, therefore, result in conservative estimates of concentrations. Although most operational models use one set of formulae or another, a few models have options to use alternative formulae or to use a "manual override" which allows actual observations of plume rise to be used directly as inputs.

It should be emphasized that the use of any of the standard formulae in complex terrain, such as coastal or mountainous terrain, often results in significant errors. Serious difficulties arise because of the effects of turbulent air flow upon plume rise, possibly resulting in either an atmospheric downwash condition, or plume impingement upon elevated terrain. An informative, practical, and quantitative discussion of plume rise and downwash can be found in Briggs (1973). A useful discussion of the options used in several operational models to treat plume rise over elevated terrain can be found in Fabrick, et al. (1977).

Meteorologic data such as temperature, wind speed and direction, and cloud cover are requisite inputs into analytical procedures for estimating atmospheric stability, which, in turn, is required in order to estimate the diffusion parameters required in Gaussian equations. (Meteorologic data are also inputs directly into Gaussian equations, as shown in figure 5-13.) In addition to being a function of atmospheric stability, diffusion parameters are also a function of the downwind distance from a discharge source. Several analytical procedures have been developed: (1) to estimate atmospheric stability from certain meteorologic data; and (2) to estimate the diffusion parameters, given atmospheric stability and downwind distance.

There are four analytical procedures for estimating atmospheric stability: Pasquill-Turner,[16] wind fluctuation, temperature gradient, and Richardson. Results produced by application of these procedures in the same context very often are not the same, particularly for nighttime periods.

Consequently, the estimation of atmospheric stability from meteorologic data continues to be the most difficult, confusing, and controversial aspect of Gaussian air quality models.

In the Pasquill-Turner procedure, the atmosphere is divided into six categories of atmospheric stability: very unstable; moderately unstable; slightly unstable; neutral; slightly stable; and moderately stable.[17] Each stability category is assumed to be applicable to both the horizontal dimension, for calculating σ_y, and the vertical dimension, for calculating σ_z. The stability category is a function of wind speed, cloud cover, and solar radiation. These data are available at U.S. Weather Bureau stations, generally found at major airports.[18] When solar radiation data are not available, time of day and season are frequently used as surrogates. Once a stability category has been determined, diffusion parameters are selected from a set of empirical curves which relate measured values of σ_y and σ_z to a stability category at a given distance downwind.

In the wind fluctuation procedure, horizontal and vertical wind standard deviations, σ_Θ and σ_e, respectively, are grouped into atmospheric stability categories, based on empirical measurements of diffusion (Cramer, et al., 1958). The stability categories are equivalent to the Pasquill-Turner categories (Slade, 1968) and diffusion parameters are selected from the empirical curves which relate σ_y and σ_z to stability, as mentioned above.

As an alternative to the wind fluctuation procedure, diffusion parameters can be calculated directly from σ_Θ and σ_e using the following formulae:

$$\sigma_y = \sigma_\theta X^a$$

$$\sigma_z = \sigma_e X^b$$

where X is the downwind distance and a and b are empirical constants which depend on whether the atmospheric temperature gradient is stable, neutral, or unstable.

The temperature gradient procedure for determining atmospheric stability is also referred to as the "delta T" method. In this procedure the change in temperature over a specified height interval is directly measured. Atmospheric stability is determined by comparing the measured temperature profile with previously determined temperature profile/stability condition combinations. Once a stability category is determined, the diffusion parameters are obtained using empirical curves, as described above.[19]

The Richardson number procedure is a direct method for determining Pasquill-Turner stability categories. The Richardson number, Ri, represents the relative importance of convective turbulence (numerator) to mechanical turbulence (deonominator). It is calculated as follows for an atmospheric layer:

$$Ri = \frac{\frac{g}{T}\left(0.01 + \frac{\Delta T}{\Delta z}\right)}{\frac{(\Delta u)^2}{(\Delta z)^2}}$$

where:

Ri = Richardson number (dimensionless);

g = gravitational constant (m/sec^2);

T = mean ambient temperature (°K);

ΔT = change in temperature over atmospheric layer (°K);

Δz = thickness of atmospheric layer (m); and

Δu = change in wind speed over atmospheric layer (m/sec).

A Richardson number is then equated to an atmospheric stability category and diffusion parameters are determined as described above.

All of the above methods for determining atmospheric stability use empirical relationships to reestimate diffusion parameters based on the Pasquill-Gifford stability curves. Therefore, the relationships developed by these methods all share several common problems. First, because the original measurements on which the curves are based were made at rather short distances downwind from the discharge source, i.e., about 1 kilometer, σ_y curves used in applications at downwind distances greater than a few kilometers are extrapolations of the actual measurements. Second, because the measurements were made in flat and gently rolling terrain, the curves are not applicable where terrain is moderately rolling or complex, e.g., alternating hills and valleys. Third, because of the difficulties associated with measuring ambient concentrations above ground level, very few direct measurements of σ_z were made in developing the curves. (In general, σ_z was computed by indirect methods.) Therefore, the accuracy of σ_z is questionable. Fourth, because the original discharges and associated measurements of ambient concentrations were both made at ground level, appropriate σ_x and σ_y for elevated discharges are not available from the original Pasquill-Gifford curves.

Differences of opinion exist among modelers with respect to the most appropriate method for estimating diffusion parameters. However, recent suggestions have been made by Pasquill (1974, 1976) for possible improvements to the original Pasquill-Gifford curves, e.g., with regard to applications in rough terrain and at greater downwind distances. Nevertheless, the basic problem remains that there are, presently, insufficient field measurements on σ_y and σ_z to draw definitive conclusions about the accuracy of the estimated diffusion parameters. For information on methods of estimating diffusion parameters see McElroy and Poller (1968) and Briggs (1973) for multiple source problems in urban areas, and Mullen, Chan and Tombach (1977) and Shearer and Minott (1977) for large elevated sources in complex terrains.

In summary, the following conclusions can be drawn with respect to the estimation of diffusion parameters. First, for application on the scale of an urban area, diffusion parameters can usually be estimated within a factor of 2 or 3. Second, at greater scales errors become larger. Third, during nighttime conditions errors are likely to be larger still, particularly in rural areas. Fourth, the variation in diffusion parameters with height is not well known. Fifth, the accuracy of the estimated diffusion parameters and hence the accuracy of the related estimates of ambient concentrations in complex terrain are low. Sixth, the phenomena related to diffusion are not at all well understood at this time and considerable additional research is warranted.

Numerically Integrated Approach

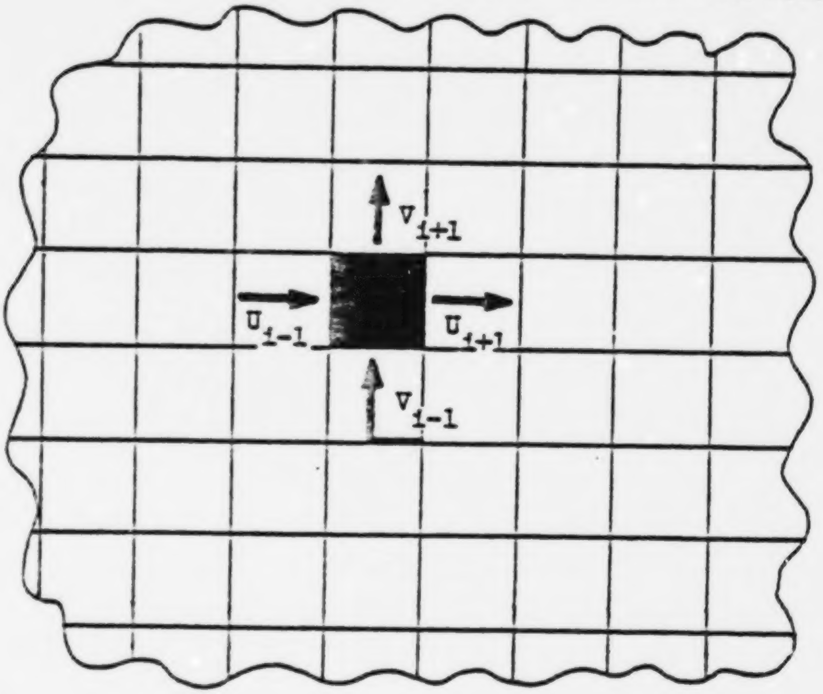
The numerically integrated approach is based on the numerical integration of equation [5-2] and is considerably more complex than either the Gaussian or volumetric approaches. Air quality models based on this approach are applicable to a number of air quality problems for which Gaussian (and volumetric models) are not suitable, because of the limiting assumptions necessary in order to integrate equation [5-2] analytically. Relevant problems include: short-term time dependent problems in which residuals discharges and meteorologic conditions vary appreciably from one time period to the next; short-term problems in which there are complicated three-dimensional variations in meteorologic conditions, e.g., wind speed and direction; and photochemically reactive problems which combine physical and chemical transformation processes. Numerical integration of the general conservation of mass or energy equation is briefly discussed in chapter 2.

There are two basic types of numerically integrated air quality models: grid area models and trajectory models. The difference between these types is the way in which discharge plumes are analyzed as they move over the land surface. Another type of numerically integrated air quality model is a photochemically reactive model. Although discharge plumes from this type of model are also analyzed on either a grid area or trajectory basis, such models in addition include explicit mathematical representations of photochemical processes which affect ambient concentrations of many important residuals, particularly photochemical oxidants. Photochemically reactive models are discussed separately in the last part of this section.

Grid area models involve numerical integration of equation [5-2] by performing mass balance calculations for a series of fixed grid area cells, as shown below in figure 5-15. (See figure 5-8 for a three-dimensional representation.) The approach is analogous to the sectioning or segmenting of a water body used in numerically integrated water quality models.

Grid area models typically estimate spatially averaged hourly concentrations of residuals for each grid area, at ground level, for specified vertical layers, or both. Ground level residuals discharges are spatially averaged over individual grid areas; elevated discharges are spatially averaged throughout vertical layers over individual grid areas. Because estimates of concentrations are spatially averaged over grid areas,

Figure 5-15. Illustration of Transport in a Grid Area Model



U and V are wind components into and out of the i^{th} cell at any given time

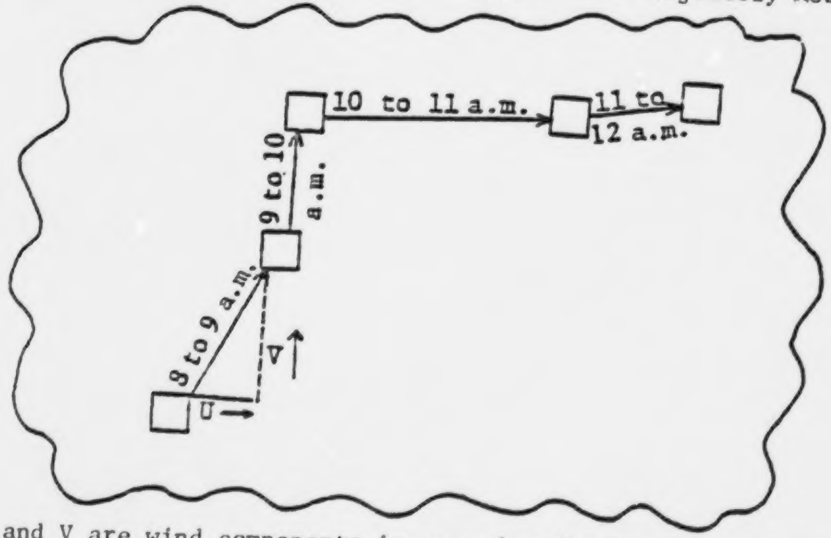
typically 1 to 5 kilometers on a side, estimates in the vicinity of large point sources are often seriously underestimated. Additional inaccuracies are introduced by simplifying assumptions that are often made, e.g., neglecting vertical advection, unless especially strong vertical movement is present, and neglecting diffusion in the x-direction. Models based on the grid area approach to numerically integrating equation [5-2] are generally preferred over models based on the trajectory approach in contexts in which there are many point sources and receptor locations.

Trajectory models involve numerical integration of equation [5-2] by performing mass balance calculations for a parcel (volume) of air as it moves over the land surface over time. The air parcel moves according to the ambient wind trajectory, as illustrated in figure 5-16, rather than remaining fixed as in the grid approach. In most cases, multiple point wind speed and direction measurements are required to determine areawide wind fields at given points in time, as inputs to the trajectory model.

Inherent in the trajectory approach are several important simplifications. First, residuals discharges are generally input into trajectory models from grid areas, just as for grid area models. Second, because the parcel moves in the mean wind direction, there can be no advective transport of residuals into the parcel from upwind sources. Third, horizontal diffusion in crosswind directions is frequently neglected. Therefore, if there are sharp, horizontal spatial differences in discharges from grid areas, neglecting horizontal diffusion can cause significant errors.

In problem contexts which consist of analyzing a few "hot spot" concentrations[20] or estimating ambient concentrations at a few receptor locations from a few large sources, trajectory models are generally more

Figure 5-16. Illustration of Transport in a Trajectory Model



U and V are wind components in x- and y-directions, respectively.

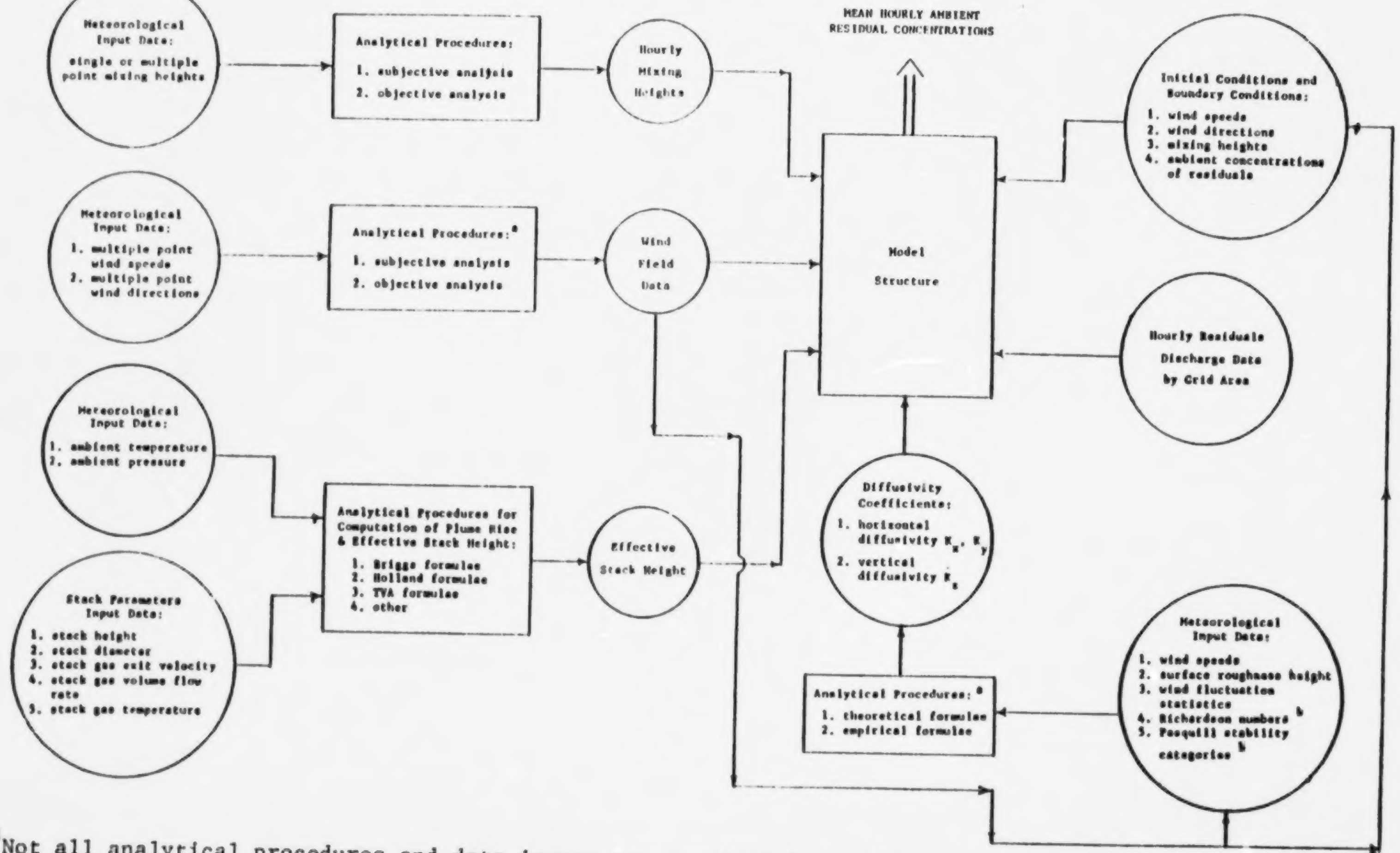
economical to use than grid area models.

Regardless of whether a numerically integrated model is based on the grid approach or the trajectory approach, certain model components are required, i.e., data inputs and analytical procedures. These components may or may not be explicitly incorporated in the model structure. Depending on the individual model, certain data may be input directly or may require processing into a form required for model inputs. Figure 5-17 illustrates these data and analytical procedures and shows how they become inputs into the numerically integrated model structure. Not all of the data inputs shown for a particular analytical procedure are required in a given model. Requisite data inputs include: various meteorologic data, residuals discharges, ambient residuals concentraitons, wind field data, and diffusivity coefficients. Wind field data and diffusivity coefficients are particularly important to explain; the other data inputs were explained in the previous section on Gaussian models.

Wind field data can be developed from wind speed and direction measurements by either interpolating and extrapolating scattered point measurements for all locations in a grid format, or using the measurements along with assumed boundary conditions to develop a two- or three-dimensional wind field for a given air parcel based on mass balance calculations. Depending on the terrain, more or fewer measurements are required. For example, complex terrain almost always requires more measurements, e.g., mountain/valley and land/water topographical features cause localized air flows which affect advection and diffusion. Note that a certain amount of observational error is always present in these measurements.

Two methods can be employed to interpolate and extrapolate wind speed and direction measurements: subjective analysis and objective analysis.

Figure 5-17. Schematic of Numerically Integrated Model Components: Data Inputs and Analytical Procedures


Meteorological Input Data: single or multiple point mixing heights
Analytical Procedures: 1. subjective analysis 2. objective analysis
Hourly Mixing Heights
Meteorological Input Data: 1. multiple point wind speeds 2. multiple point wind directions
Analytical Procedures:ᵃ 1. subjective analysis 2. objective analysis
Wind Field Data
Meteorological Input Data: 1. ambient temperature 2. ambient pressure
Stack Parameters Input Data: 1. stack height 2. stack diameter 3. stack gas exit velocity 4. stack gas volume flow rate 5. stack gas temperature
Analytical Procedures for Computation of Plume Rise & Effective Stack Height: 1. Briggs formulae 2. Holland formulae 3. TVA formulae 4. other
Effective Stack Height
MEAN HOURLY AMBIENT RESIDUAL CONCENTRATIONS
Model Structure
Initial Conditions and Boundary Conditions: 1. wind speeds 2. wind directions 3. mixing heights 4. ambient concentrations of residuals
Hourly Residuals Discharge Data by Grid Area
Diffusivity Coefficients: 1. horizontal diffusivity K_x, K_y 2. vertical diffusivity K_z
Analytical Procedures:ᵃ 1. theoretical formulae 2. empirical formulae
Meteorological Input Data: 1. wind speeds 2. surface roughness height 3. wind fluctuation statistics 4. Richardson numbersᵇ 5. Pasquill stability categoriesᵇ

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[a] Not all analytical procedures and data inputs are required for a given operational model.

[b] These in turn are calculated from other input data.

In subjective analysis a meteorologist familiar with the region assigns wind speeds and directions to locations based on a combination of available data and his own experience. In objective analysis a set of consistent rules is used to process the measured data. Objective analysis methods range from the very simple to the complex. For example, a simple method frequently used to interpolate two-dimensional wind speed and direction data at a given location is to apply an inverse square weighting of the distance from the specified location to all measured observations.

Three-dimensional wind fields developed based on assumed or given boundary conditions and mass balance calculations assume that the mass of air entering a specified volume is equal to the mass of air flowing out. Such wind fields enable consideration of changes in wind speed and direction with height, referred to as wind shear. Wind shear is important to consider in contexts in which elevated discharges occur or complex terrain exists. For a discussion of some of the methods for deriving wind fields see Fabrick, et al. (1977).

Diffusivity coefficients, K_x, K_y, and K_z, shown in figure 5-17, are analogous to the diffusion parameters used in Gaussian models discussed earlier. They represent the diffusion process in a similar way and permit the effects of three-dimensional variations in wind speed and terrain on diffusion processes to be considered. In some models, diffusivity coefficients may be exogenous inputs. However, most operational models contain subroutines which compute the coefficients based on the variables shown in figure 5-17. Methods for computing the coefficients vary considerably, ranging from empirical to rather theoretical formulations, such as the Monin-Okukhov Stability Theory. This variation in methods has resulted in significant differences in the input data requirements for estimating diffusivity coefficients in different models. For a discussion and comparison of some of the methods used see Fabrick, et al. (1977).

Photochemically reactive air quality models differ from other numerically integrated air quality models in that they include explicit mathematical formulations to take into account photochemical processes which affect ambient concentrations of many important residuals. Photochemical processes and the air quality problems which they affect were discussed in the first two sections of the chapter.

In photochemically reactive models, mathematical expressions for relevant photochemical reactions are incorporated into the "R" term in the basic conservation of mass and energy equation, equation [5-2] in this chapter. These reactions are used to estimate the amounts of various residuals and other constituents which are either produced or destroyed by photochemical reactions in a specified control volume or over time. As indicated earlier, literally hundreds of reactions which form harmful photochemical oxidants take place in the atmosphere. Because of an incomplete understanding of these processes, the usual lack of sufficient discharge data, and the sheer volume of computations which would be required, photochemically reactive models include only the more important reactions and lump many reactions together, depending on the constituents of interest. Existing models typically include from fifteen to fifty reactions. For example, table 5-1 shows the sixteen photochemical reactions and their related rate constants which are used in the DIFKIN models.[21] For additional information on modeling photochemical reactions see Frielander and Seinfeld (1969), Hecht, et al. (1974), Demerjian, et al. (1974), and MacCracken and Sauter (1975).

In order to illustrate how photochemical reactions are incorporated in the basic conservation of mass and energy equation, consider the following

Table 5-1. Photochemical Reactions and the Rate Constants Used in the DIFKIN Model

Photochemical Reaction	Rate Constant, $pphm^{-1}$ min^{-1}
1. $HV + NO_2 = NO + O_3$	1×10^{-4}
2. $NO + O_3 = NO_2 + O_2$	2.67×10^{-1}
3. $O + HC = 8RO_2$	1×10^{-6}
4. $OH + HC = 8RO_2$	1×10^{2} [a]
5. $RO_2 + NO = NO_2 + 0.125 \times OH$	1×10^{3}
6. $RO_2 + NO_2 = PAN$	2×10^{0}
7. $OH + NO = HNO_2$	1.5×10^{1}
8. $OH + NO_2 = NHO_3$	3×10^{1}
9. $O_3 + HC = RO_2$	4×10^{-5}
10. $HV + HONO = OH + NO$	3.7×10^{-7}
11. $NO_2 + O_3 = NO_3 + O_2$	5×10^{-5}
12. $NO_3 + NO_2 = N_2O_5$	4.5×10^{1}
13. $N_2O_5 = NO_3 + NO_2$	1.4×10^{1}
14. $N_2O_5 + H_2O = 2HNO_3$	6.05×10^{1}
15. $NO + NO_2 + H_2O = 2HNO_2$	1×10^{-5}
16. NO_2 + PARTICLES = PRODUCTS	1×10^{-3}

[a] Varies depending on the initial ratio of HC to NO_x

mechanism posited for the formation of ozone (O_3) by Miksad, et al. (1977):

$$NO + O_3 \xrightarrow{k_1} NO_2 + O_2$$

$$NO_2 \xrightarrow{k_2} NO + O_3$$

where k_1 and k_2 are rate constants.[22] Given the reaction mechanisms shown above, the "net" rate of change of each constituent can be represented as a partial differential equation:

$$\text{[5-6]} \qquad \begin{aligned} \frac{\partial(NO)}{\partial t} &= -k_1(NO)(O_3) + k_2(NO_2) \ ; \\ \frac{\partial(NO_2)}{\partial t} &= k_1(NO)(O_3) - k_2(NO_2) \ ; \\ \frac{\partial(O_3)}{\partial t} &= -k_1(NO)(O_3) + k_2(NO_2) \ . \end{aligned}$$

Given appropriate values for k_1 and k_2, these equations yield estimates of the amount of ozone, O_3, which will be produced in a specified volume over time, given the net amount of each constituent present in the volume over time, i.e., the amount initially in the volume plus inflows minus outflows.

Combining each of the equations in [5-6] with a conservation of mass and energy equation for each constituent, to account for inflows and outflows of the constituent, results in a system of three simultaneous equations which constitute a simple photochemically reactive model. These equations are:

$$\text{[5-7]} \qquad \frac{\partial(NO)}{\partial t} = \overbrace{-U_x \frac{\partial(NO)}{\partial x}}^{\text{Advection}} + \overbrace{K_y \frac{\partial^2(NO)}{\partial y^2} + K_z \frac{\partial^2(NO)}{\partial z^2}}^{\text{Diffusion}} \overbrace{- k_1(NO)(O_3) + k_2(NO_2)}^{\text{Photochemical Reaction}} \ ;$$

[5-7] Continued

$$\frac{\partial(NO_2)}{\partial t} = \overbrace{-U_x\frac{\partial(NO_2)}{\partial x}}^{\text{Advection}} + \overbrace{K_y\frac{\partial^2(NO_2)}{\partial y^2} + K_z\frac{\partial^2(NO_2)}{\partial z^2}}^{\text{Diffusion}} + \overbrace{k_1(NO)(O_3) - k_2(NO_2)}^{\text{Photochemical Reaction}} ;$$

$$\frac{\partial(O_3)}{\partial t} = \overbrace{-U_x\frac{\partial(O_3)}{\partial x}}^{\text{Advection}} + \overbrace{K_y\frac{\partial^2(O_3)}{\partial y^2} + K_z\frac{\partial^2(O_3)}{\partial z^2}}^{\text{Diffusion}} \overbrace{- k_1(NO)(O_3) + k_2(NO_2)}^{\text{Photochemical Reaction}}$$

where: U_x = mean wind speed in the x-direction (m/sec.);

t = time (sec.);

K_y and K_z = diffusivity coefficients for the y- and z-directions, respectively (m/sec.); and

k_1 and k_2 = rate constants.

Note that the equations in [5-7] neglect diffusion in the x-direction, assume the mean wind direction is in the x-direction, and neglect advection in the vertical, y, direction.

These equations [5-7]--three nonlinear simultaneous equations with three unknowns, NO, NO_2, and O_3--represent a significant computational problem when they must be solved for a large number of grid areas. When additional constituents are considered, the computational problem becomes correspondingly larger. When N constituents are considered for M grid areas, N x M simultaneous equations must be solved. Consequently, depending on the problem context--the number of constituents and grids considered--the advection and diffusion terms are frequently "decoupled" from the chemical reaction terms and separately solved numerically. The concentrations computed for each grid area due to advection and diffusion then become inputs into the chemical reaction equations. This decoupling approach significantly reduces the computational problem.

For information on specific photochemically reactive models, see Appendix A. For additional information on photochemical reactions, see Record, et al. (1975), and National Research Council (1977).

Statistical and Proportional Approaches

Statistical approaches have had, and continue to have, considerable use in the analysis of atmospheric systems. However, there are two problems with the statistical approach: (1) it does not explain causal relationships; and (2) the range over which a statistical model can make predictions is generally limited to the range represented by the sample on which the statistical analysis is based. Nevertheless, because of their simplicity, models based on the statistical approach continue to have utility in certain contexts. Examples of such contexts are: (1) where a first, crude analysis is required; and (2) where the detailed quantitative data necessary to apply a more complex model, i.e., one based on the conservation of mass and energy approach, are not available.

Similarly, an even simpler type of model--the proportional model--has also been used in many contexts because of its simplicity and because of expediency. Proportional models generally provide even less information than statistical models, because they assume that the ambient concentration at any given location in a region is proportional simply to the percentage increase or decrease in total residuals discharges in the region. Proportional models were used by many jurisdictions in preparing the first implementation plans which were mandated under the Clean Air Act.

Statistical Approach

The statistical approach for analyzing atmospheric systems is essentially the same as the general statistical approach for analyzing natural systems described in chapter 2. The principal statistical method employed is regression analysis, although other methods have also been applied.[23] Therefore, this section will only briefly illustrate the application of regression analysis to the analysis of atmospheric systems.[24]

In regression analysis a dependent variable, Y, is expressed as a function of some number of independent variables, X_i, each times a coefficient, B_i, plus a random disturbance term, E, assuming some structural form, e.g., linear, semi-log, log-log. The most common form of regression equation is multiple linear, the term "multiple" indicating that more than one independent variable is included in the equation. This equation is of the form: $Y = a + B_iX_i + \ldots + B_nX_n + E$, where a is a constant (the intercept).

In order to apply regression analysis to an ambient air quality problem, it is important that the specific problem to be addressed, the natural phenomena involved, and the limitations of available data be well understood. A certain amount of ingenuity is also generally required to make the best use of the available data. For example, consider the time period of analysis. Depending on the time period chosen, available data can be aggregated into a larger or smaller number of independent observations. The more observations included, generally the more statistically valid are the results. If annual averages were to be used, it is unlikely that a sufficient number of years of data would be available. If seasonal averages were used, more observations would be available; if monthly averages used, still more; and so on. The analyst must decide the time period which makes the most sense, given the phenomena involved and the problem of concern, plus feasibility of application with respect to the data available. Ingenuity is also required in the choice of the independent variables to include in the regression.

Should both meteorologic and residuals discharge variables be included? Which specific variables make the most sense given the phenomena of concern and the problem context, i.e., with respect to REQM? The two examples which follow illustrate how some of these concerns may be considered.

Basta, Lounsbury, and Bower (1978) developed multiple linear regression models for sulfur dioxide, SO_2, and total suspended particulates, TSP, for application to an urban area surrounded by mountains. Their objective was to construct a simple model which would enable preliminary evaluation of various physical measures for improving ambient air quality, in terms of their relative costs and impacts on ambient air quality. The choice of a multiple linear regression form was based on an assessment of available analytical resources, including data, and an examination of the physical and meteorologic characteristics of the region. For example, analysis of available monitoring data showed relatively small differences in mean meteorologic conditions such as wind speed, wind direction, and precipitation, within the region being analyzed. The multiple linear regression models posited were of the following form:

$$Y_S \text{ or } Y_{TSP} = B_1 + B_2X_1 + B_3X_2 + B_kX_n + E,$$

where: Y_S or Y_{TSP} = mean ambient concentration of SO_2 and TSP, respectively, at ground level;

$X \ldots X_n$ = meteorologic and residuals discharge variables;

$B_1 \ldots B_k$ = coefficients to be estimated; and

E = random disturbances.

Based on observed differences in ambient air quality for different periods of the year, three climatic periods were identified for separate analysis: winter, spring/fall, and summer. Each period contained four months and was divided into seven-day intervals. Given three years of data, 52 observations could be constructed for each variable included in the regression, for each climatic period.

Four meteorologic variables and eight residuals discharge variables were included in the regressions. These meteorologic variables were:

X_1 = precipitation per day (mm);

X_2 = average wind speed per day (m/sec.);

X_3 = meteorologic stability per day,
five ordinate classes:

1. markedly cyclonic,
2. cyclonic,
3. undefinable,
4. anticyclonic,
5. markedly anticyclonic; and

X_4 = duration of inversion per day,
four classes:

0. 0 hrs.,
1. 0 hrs. $< X_4 \leq$ 8 hrs.
2. 8 hrs. $< X_4 \leq$ 16 hrs.,
3. 16 hrs. $< X_4 \leq$ 24 hrs.

The residuals discharge variables were defined in terms of kilograms per day discharged from:

X_5 = chemical industry;

X_6 = metal processing industry;

X_7 = pulp and paper industry;

X_8 = all other industry;

X_9 = power plants;

X_{10} = single-flat residences;

X_{11} = multi-flat residences;

X_{12} = all other activities.

Seven-day averages were computed for each of the variables. Regression coefficients were estimated for each climatic period--for SO_2 and TSP separately--using a "backward stepwise" least squares regression routine in conjunction with a principal components subroutine.

Based on standard statistical tests, e.g., coefficient of determination, F test, Student's T test, and the Durbin-Watson statistic for autocorrelation, the regression equations estimated for the winter period were found to be sufficiently significant to be used to investigate the effects of different physical measures to improve air quality. However, Basta, Lounsbury, and Bower stress that careful interpretation is an essential ingredient in the use of statistical models; if the results cannot be explained in terms of underlying physical and technological processes, the model should not be used.

Another example of the application of regression methods for analyzing ambient air quality is the recpetor-oriented model developed by Roberts and Croke (1970). This model is termed a receptor-oriented model because the dependent variable is ambient concentration at a specific location. In a given region, an equation such as that shown below would be estimated for each receptor location for which ambient concentration data were available. This is in contrast to the regression equations described in the illustration above, which yield estimates of ambient concentrations for the region as a whole.

The form of the regression equation posited by Roberts and Croke is:

$$Y = C_o + C_1Q_1 + C_2Q_2 + \sum_{i=1}^{n} K_iQ_i$$

where: Y = concentration at a given receptor location (g/m^3);

C_o = background concentration of residual of interest, (g/m^3);

Q_1 and Q_2 = residuals discharges for individually specified source categories

K_iQ_i = residuals discharges attributed to n other large individual point sources; and

C_1 and C_2 = coefficients to be estimated.

In applying this equation, the data must be stratified by wind direction, wind speed, and time of day.

A point of interest is that Roberts and Croke indicate that the coefficients C_1, C_2, and K_i represent the $\frac{1}{\sigma_y \sigma_z}$ term plus the contribution of the exponential term in the Gaussian type diffusion equation described in the previous section. As do Gaussian receptor-oriented models, the Roberts and Croke regression equation results in estimates of the contributions from various sources in a region to ambient concentrations at a specified location. It remains to be seen which approach would be more accurate in any given context. Lack of data is a severe constraint to the application of the Roberts and Croke equation, as it is for most regression equations. Gaussian models require fewer ambient concentration data.

Proportional Approach

Proportional models can be either "rollforward" or "rollback", and the relationship between the dependent and independent variables either linear or nonlinear. The terms rollforward and rollback relate to the specification of the dependent variable in the relationship posited. In rollforward models the dependent variable is ambient concentration of a residual at a specified location at some future point in time. Given the existing (present) concentration of a residual at a specified location at time t1, background concentration, discharge of the residual in the region at time t1, and an estimate of projected discharge of the residual at time t2, the concentration for the location at time t2 can be estimated. The rollforward formulation is:

$$C_{t2} = \left[C_{t1} - B\right]\frac{Q_{t2}}{Q_{t1}} + B \tag{5-8}$$

where:
C = concentration (g/m^3);
t = time;
Q = residuals discharge; and
B = background concentration (g/m^3).

Equation [5-8] represents a linear, rollforward, proportional model.

Alternatively, in the rollback form of the linear proportional model, equation [5-8] is rearranged so that the dependent variable is the percent reduction in discharges of a residual in a region required to reduce the ambient concentration existing at a location at time t1 to a prespecified level at time t2, for example, the ambient standard. The linear rollback form of equation [5-8] is:

$$R = 1 - \frac{Q_{t2}}{Q_{t1}} \times 100\% = \frac{C_{t2} - B}{C_{t1} - B} \times 100\%$$

where:
R = percent reduction in residuals discharge;
C_{t2} = a prespecified ambient standard (g/m^3); and

all other variables are as specified for equation [5-8].

Nonlinear rollback and rollforward models have been used primarily to estimate oxidant concentrations. One form of this relationship is the Appendix J curve of EPA regulation 40 CFR 51. For any given urban area, the areawide, mean daily concentration of hydrocarbons between 6:00 a.m. and 9:00 a.m. can be plotted against the daily maximum oxidant concentration--for any single monitoring station--for the months of interest.

Figure 5-18 shows the Appendix J curve for the nonlinear hydrocarbon relationship, based on data from five cities.

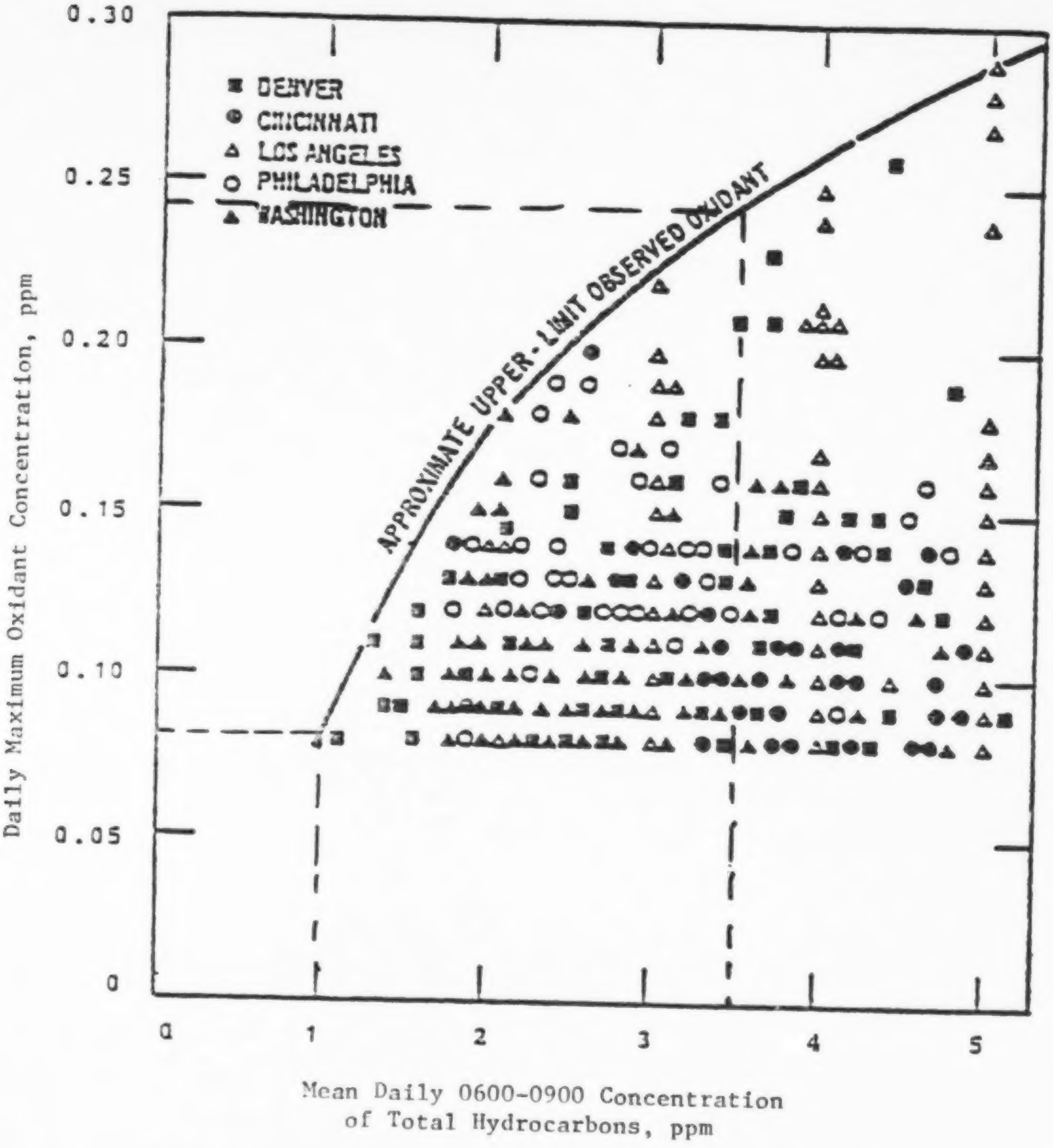
As an example, consider a situation where it is desired to reduce the daily maximum oxidant concentration in a region from 0.24 ppm to 0.08 ppm, which represents about a 67 percent reduction. According to the curve shown in figure 5-18, hydrocarbon concentration would have to be decreased from about 3.5 ppm to about 1 ppm, a reduction of about 72 percent. If it is then assumed that the relationship between ambient hydrocarbon concentration and discharges is linear, the linear rollback relationship can be used to estimate the amount that hydrocarbon discharges in the region would have to be reduced to achieve the specified oxidant concentration, i.e., 0.08 ppm. This procedure can also be used in the reverse, i.e., to estimate oxidant concentrations given a projected level of hydrocarbon discharges for a future time period.

It is important to emphasize that the proportional approaches described above are very limited, for example, because of the lack of spatial resolution and because of the assumption that oxidant concentrations depend solely on hydrocarbons.[25] For a discussion of the limitations of these approaches and how they may be used to provide useful information in certain contexts, see Record, et al. (1975).

SELECTING AN APPROPRIATE AIR QUALITY MODEL

This section has two purposes. The first is to assist an analyst in determining whether or not the proposed air quality analysis is feasible. The second is to assist the analyst in the selection of an air quality model best suited for application in the given context, based on other relevant criteria.

Figure 5-18. Plot of Daily Maximum 1-Hour Oxidant Concentrations Versus Average Hydrocarbon Concentrations for Five U.S. Cities



Source: U.S. Environmental Protection Agency, Guidelines for Air Quality Maintenance Planning and Analysis, Volume 12: Applying Atmospheric Simulation Models to Air Quality Maintenance Areas EPA-450/4/-74-013 (Research Triangle Park, North Carolina, EPA, 1974).

This section corresponds to the section on setting up the natural systems analysis in chapter 2. In chapter 2 a logical sequence of steps was described which could be followed to ascertain what types of natural systems analysis to undertake in any given context. Six steps were identified and defined in table 2-3. The fourth step in the sequence related to determining the feasibility of carrying out the natural systems analysis specified in the previous three steps; the fifth step related to selecting an NSM for application based on relevant evaluation criteria. The material in this section is therefore an extension of these two steps, given a context in which an analysis of the atmospheric system is required.

Five elements comprise this section: (1) a listing of air quality models, both operational and nonoperational, known as the population table; (2) a table which relates air quality problem characteristics to the models in the population table, referred to as the problem table; (3) a flow diagram which indicates how to select an appropriate air quality model using the material contained in the chapter, referred to as a selection procedure; (4) a discussion of the characteristics which are used to summarize each of the operational air quality models, referred to as model characteristics; and (5) summaries of the characteristics of operational air quality models. The fifth element, in the form of model summary tables for 33 air quality models, is contained in Appendix A.

Population of Air Quality Models

Table 5-2 lists the air quality models which were reviewed in preparing this chapter. The majority of air quality models currently in general use is represented in the population. In cases where a number of models were essentially the same, only one or two models were included as being

Table 5-2. Population of Air Quality Models for Potential Application in REQM Analysis

Model Category/Model Name	I	II	Commonly Used Acronym	Originator /Contact Person
Conservation of Mass Models				
• Volumetric				
Gifford-Hanna*	X		---	Frank Gifford & Steve Hanna. Atmospheric Diffusion Lab., Oak Ridge Nat'l. Lab., Oak Ridge, Tenn.
Gifford-Hanna Photochemical*	X		---	" "
• Gaussian				
Air Quality Display Model*		P	AQDM	TRW Systems Group under contract to National Air Pollution Control Admin. (presently EPA) Mr. Bruce Turner. Contract Officer*
Climatological Display Model*		P	CDM	Meteorology Lab., EPA Research Triangle Park N.C. (UNAMAP Series)
Air Quality Submodel of the Transportation and Air Shed Simulation Model[b]*		A,P		Norm Cooper, Office of Environmental Affairs. U.S. Dept. of Transportation, Washington, D.C.
COPOLLUT		A	---	C.R. Gebhardt. Ohio Dept. of Transportation, Columbus, Ohio
California Line Source Dispersion Model*	X		CALINE 2	Mr. Andy Ranzieri. Calif. State Div. of Highways, Sacramento. Calif.
EPA HIWAY*	X		HIWAY	Meteorology Lab., EPA, Research Triangle Park, N.C. (UNAMAP Series)
Point, Area, Line Source Model*		P	PAL	Bruce Turner & William B. Petersen, Meterology Lab., EPA, Research Triangle Park, N.C.
Single Source Model*		P	CRSTER	Russell Lee, et al., Source Receptor Analysis Branch, Office of Air Quality Planning & Standards, EPA, Durham, N.C.
Air Pollution Research Advisory Committee 1A*		A	APRAC 1A	R.C. Manusco & F.L. Ludwig, Stanford Research Institute, Menlo Park, Calif., (UNAMAP Series)
PTMAX*		P	PTMAX	Meteorology Lab., EPA, User Network of Applied Models of Air Pollution (UNAMAP Series)
PTDIS*		P	PTDIS	" "
PTMTP*		P	PTMTP	" "
Real-Time Air Pollution Model		P	RAM	Mr. Bruce Turner & Ms. Joan Novak. Meteorology Lab., EPA, Research Triangle Park, N.C (to be included in UNAMAP Series)
Gaussian Evaluation Model*		P	GEM	A. Fabrick, R. Sklarew,[c] J. Wilson, Science Applications, Inc., Westlake Village, Calif.
Argonne Puff*		P	---	E.J. Croke, J.J. Roberts, et al., Energy & Environmental Div., Argonne National Lab., Argonne, Ill.
Stanford Research Institute		P	SRI	Ron Ruff, Stanford Research Institute, Palo Alto, Calif.
Great Lakes University of Wisconsin at Milwaukee Meso Meteorological Project[h]	X		GLUMP	Walter Lyons, University of Wisconsin at Milwaukee[d]
VALLEY*		P	---	Edwart Burt, Source Receptor and Analysis Branch, Office of Air Quality Planning & Standards, EPA, Durham, N.C.
Oak Ridge Fog and Drift*		P	ORFAD	John Wilson, Oak Ridge National Lab., Oak Ridge, Tenn.
Atmospheric Transport Model*		P	---	Walter Culkowski[e] and Malcolm Patterson,[f] Oak Ridge National Lab., Oak Ridge, Tenn.
Drift Transport Cooling Tower	X		---	Gunter Schrecker, Environmental Systems Corp., Knoxville, Tenn.[g]
The Research Corp. of New England Cooling Tower*		P	TRC	Norm Bowne. The Research Corp. of New England, Wethersfield, Conn.

continued . . .

Table 5-2. Population of Air Quality Models for Potential Application in REQM Analysis (Continued)

Model Category/Model Name	I	II	Commonly Used Acronym	Originator /Contact Person
• Gaussian				
Texas Episodic Model*		P	TEM	John Christiansen, Data Processing Div., Texas Air Control Board, Houston, Texas[h]
Texas Climatological Model*		P	TCM	" "
• Numerically Integrated				
International Business Machines Air Quality 1&2 *		W	IBMAQ 1&2	Danny Shieh, International Business Machines, Inc., San Jose, Calif.
INTERA		W	INTERA	Ron Lantz, INTERA, Environmental Consultants, Ltd., Houston, Tx.
Atmospheric Diffusion Particle-In-Cell		W	ADPIC	Mike MacCracken & Rolf Lange, Lawrence Livermore Lab., Livermore, Calif.
Scavenging Model Incorporating Chemical Kinetics	X[i,j]		SMICK	J.M. Hales, et al., Atmospheric Sciences Section, Battelle N.W. Lab., Richland, Wash.
Atmospheric Carbon Monoxide Simulation Program*		W	ACSOP	Robert Carlson & William Norton,[k] Univ. of Alaska, Fairbanks, Alaska
Livermore Regional Air Quality I*		W	LIRAQ I	Mike MacCracken, Lawrence Livermore Lab., Livermore, Calif.
Livermore Regional Air Quality II		W	LIRAQ II	" "
Reactive Plume Model*	X		RPM	Mei-Kao-Liu, Systems Applications, Inc., San Rafael, Calif.
Chemically Reactive Powerplant Plume Model (not coded)			---	R.W. Miksad,[l] K.K. DeBewers,[m] and J.R. Brock,[n] Austin, Texas
Integrated Model for Plume and Atmospherics in Complex Terrain*		W	IMPACT	A. Fabrick, R. Sklarew,[c] J. Wilson, Science Applications, Inc., Westlake Village, Calif.
Brookhaven National Laboratory Long and Short Range Air Quality Model"		W	BNL	Ron Meyers, Brookhaven National Lab., Atmospheric Sciences Sec., Upton, N.Y.
Statistical Turbulent Incompressible Fluid Flow	X		STIFF-3	James Taft, Systems, Science & Software, La Jolla, Calif.
Westinghouse Cooling Tower	X		---	Amiran Roffman & Ralph Grimble, Environmental Systems Dept., Westinghouse Electric Corp., Monroeville, Pa.
Reactive Environmental Simulation Model*		A	REM & REM 2	Peter Drivas, Pacific Environmental Services, Inc., Santa Monica, Calif.
Diffusion Kinetics Model*		A	DIFKIN	Alan Eschenroeder, Environmental Research & Technology, Inc., Santa Barbara, Calif.
Center for the Environment and Man			CEM	Joseph Pandolfo, Center for the Environment & Man, Hartford, Conn.
Systems Application, Inc. Photochemical*		A	SAI	Steven Reynolds & Philip Roth, Systems Applications, Inc., San Rafael, Calif.
Regional Transport Model of Atmospheric Sulfates[h]	X		---	K.S. Rao,[e] T. Thompson,[o] & B.A. Egan[o]
Numerical Examination of Urban Smog		W	NEXUS	R. Sklarew,[c] A. Fabrick,[p] J. Prager, Systems, Science & Software, Inc., La Jolla, Calif.
Other Models				
• Proportional				
Rollback Appendix J*	X		APPENDIX J	U.S. Environmental Protection Agency Regulation (40CFR51)
• Statistical				
Croke and Roberts*	X		---	F.J. Croke and J.J. Roberts, Energy & Environmental Systems Div., Argonne, Ill.
Repro Model*	X		---	Technology Service Corp., Santa Monica, Calif. under contract to EPA, National Environmental Research Center, Research Triangle Park, N.C.[q]

continued . . .

Table 5-2. (Continued)

KEY

*	indicates model is operational
I	indicates a pure air quality model
II	indicates a combination air quality model, including one or more of:
A	residuals discharge submodel
P	plume rise submodel
W	windfield submodel

NOTES

1. For references on models see Appendix B.
2. Footnotes

[a] Air Quality Display Model presently available from the National Technical Information Service, Springfield, Va. (Pub. No. PB-189 194).

[b] One subroutine of model addresses air quality portion of problem.

[c] Present affiliation: Form and Substance, Inc., Westlake Village, Cal.

[d] Present affiliation: MESOMET Inc., Minneapolis, Minn.

[e] Atmospheric Turbulence and Diffusion Lab., Oak Ridge, Tenn.

[f] Computer Sciences Division

[g] Present affiliation: University of Tennessee, Knoxville, Tenn.

[h] Present contact: Carol Ransom, Data Processing Division, Texas Air Control Board

[i] Denotes that model is nonoperational at present in sense defined.

[j] Contains wet chemistry model.

[k] Resource Management Association, Lafayette, Cal.

[l] Atmospheric Sciences Group, University of Texas, Austin, Texas

[m] Radian Corporation

[n] Chemical Engineering Department, University of Texas, Austin, Texas

[o] Environmental Research and Technology, Inc., Concord, Mass.

[p] Present affiliation: Science Applications, Inc., Westlake Village, Cal.

[q] Present contact: Meteorology Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina

representative of a generic class of models. Three additional comments concerning the population are in order.

First, because of their limited applicability in most REQM contexts, physical scale models have not been considered herein and hence do not appear in the table. However, it should be recognized that there is a long history of use of physical scale models for analyzing certain types of air quality problems, for example, stack design, and that--in some contexts--physical scale models would be preferred to the models presented herein.

Second, the second and third columns of table 5-2 indicate whether or not the model as conceived by its originator--and presumably in its presently available form--contains subroutines for generating and/or processing certain requisite data inputs. If a model contains no such subroutines it is termed a "pure air quality model" and an X is indicated in colume I. If a model contains one or more subroutines, one or more of the indicators P, A, and W will appear in the column headed II. P, A, and W signify, respectively, subroutines relating to: a plume rise submodel; a residuals discharge submodel; and a windfield submodel. As can be seen from the table, many models contain at least one subroutine.

Third, of the 47 air quality models listed in the table, 33 were found to be operational. These are identified on the table with asterisks. As defined previously, an air quality model must have two attributes to be considered operational. One, it must have been successfully applied to, and verified for, at least one application and be capable of being used to model another different, but roughly similar, atmospheric system without extensive modification. Two, sufficient documentation about the model must be available to enable a user to apply it in a location other than that for which it has been verified.

Relating Problems to Models

Table 5-3 relates the air quality models identified in table 5-2 to the characteristics of the major air quality problems discussed in the first section of this chapter. The purpose of this table is to provide an efficient manner in which to review the capabilities of both operational and nonoperational models to address typical air quality problems which are likely to be encountered in various REQM contexts.

Based on this table, an analyst can develop two sets of information. One, for any given problem characteristic or set of characteristics, a number of models which can address these aspects of a problem can be identified. Two, for any given model identified in the table, the problems it can address can be easily identified, and other models capable of addressing the same problems identified. However, no information about how and with what level of specificity a model can analyze a problem can be obtained from the table. Therefore, table 5-3 must be used in conjunction with the model summary tables contained in appendix A. Given a number of models of interest identified by means of table 5-3, the model summaries in appendix A provide the requisite details about each model. If a model is nonoperational, no summary table will be found in appendix A. However, appendix B, Annotated Bibliography for Air Quality Models, can be consulted to ascertain what information concerning the model has been identified in the course of preparing this chapter. Table 5-3, the model summary tables, and appendix B are integral parts of the procedure for selecting an appropriate air quality model.

Table 5-3. Air Quality Models and Their Relevance to Specific Problems

		PROBLEM CHARACTERISTICS																																										
		RESIDUAL																			SOURCE						RECEPTOR				TERRAIN						TIME				SCALE			
	MODEL TYPE/MODEL DESIGNATION	SO_2	Suspended Particulates	NO_x	HC_x	CO	Oxidants	Toxic Metals	Nutrients or Salts	Water Vapor	Sensible Heat	Radioactivity	Pesticides	Aeroallergens	Fugitive Dust	Surface Deposition (dry)	Surface Deposition (wet)	Acid Rain Deposition	Sulfates	Cooling Systems	Single Point Source	Multiple point sources	Line Source[a]	Area Sources	Ground-Level Discharge	Elevated Discharge	Point Receptor	Area Receptor	Ground-Level Receptor	Elevated Receptor	Smooth or Gently Rolling	Rough Urban	Shore or Coastal Area	Valley or Basin	Hilly or Mountainous	Forest	Steady-State	Dynamic	Long-Term	Short-Term	Up to a Few Km	Few Km to 50 Km or so	50 Km to 200 Km or so	Greater than 200 Km
CONSERVATION OF MASS	VOLUMETRIC																																											
	Gifford-Hanna	●	●	●	●	●	●																	●	●			●	●			●					●		●	●		●		
	Gifford-Hanna Photochemical				●		●																	●	●			●	●			●						●		●		●		
	GAUSSIAN																																											
	Air Quality Display Model	●	●																			●		●	●	●	●		●			●					●		●	●	●	●		
	Climatological Display Model	●	●																			●		●	●	●	●		●			●					●		●	●	●	●		
	TASSIM Submodel[a, c]	●	●	●	●	●		●														●		●	●	●	●		●			●					●		●	●	●	●		
	COPOLIT[a]					●																	●		●		●		●		●						●			●	●			
	CALINE 2[a]			●	●	●																	●	●	●	●	●		●		●	●					●		●		●			
	EPA HIWAY[a]			●	●	●		●															●		●		●		●	●	●	●					●			●	●			
	PAL[a]	●	●	●	●	●		●													●	●	●	●	●	●	●		●	●	●						●			●	●			
	CRSTER	●	●	●				●													●				●	●	●		●	●	●	●					●		●	●	●	●		
	APRAC 1A[a]					●																	●	●	●		●		●		●	●					●		●	●	●	●	●	
	PTMAX	●	●	●	●	●		●		●	●									●	●				●	●	●		●	●	●	●					●			●	●	●		
	PTDIS	●	●	●	●	●		●		●	●									●	●				●	●	●		●	●	●	●					●			●	●	●		
	PTMTP	●	●	●	●	●		●		●	●									●		●			●	●	●		●	●	●	●					●			●	●	●		
	RAM	●	●	●	●	●		●													●	●		●	●	●	●		●	●	●	●					●			●	●	●		
	GEM	●	●	●																	●	●			●	●	●		●	●	●	●		●	●	●	●			●	●	●		

Table 5-3. Air Quality Models and Their Relevance to Specific Problems (Continued)

		PROBLEM CHARACTERISTICS																																										
		RESIDUAL																			SOURCE						RECEPTOR				TERRAIN						TIME				SCALE			
	MODEL TYPE/MODEL DESIGNATION	SO_2	Suspended Particulates	NO_x	HC_x	CO	Oxidants	Toxic Metals	Nutrients or Salts	Water Vapor	Sensible Heat	Radioactivity	Pesticides	Aeroallergens	Fugitive Dust	Surface Deposition (dry)	Surface Deposition (wet)	Acid Rain Deposition	Sulfates	Cooling Systems	Single Point Source	Multiple point sources	Line Source [a]	Area Sources	Ground-Level Discharge	Elevated Discharge	Point Receptor	Area Receptor	Ground-Level Receptor	Elevated Receptor	Smooth or Gently Rolling	Rough Urban	Shore or Coastal Area	Valley or Basin	Hilly or Mountainous	Forest	Steady-State	Dynamic	Long-Term	Short-Term	Up to a Few km	Few km to 50 km or so	50 km to 200 km or so	Greater than 200 km
CONSERVATION OF MASS	GAUSSIAN																																											
	Argonne Puff	●	●																		●	●		●	●	●	●		●	●	●	●						●		●	●	●		
	SRI	●	●	●																	●	●				●	●		●	●		●			●	●		●		●	●	●		
	VALLEY	●	●	●				●													●	●		●	●	●	●		●	●	●	●		●	●	●	●		●	●	●	●		
	Oak Ridge Fog and Drift								●							●				●	●				●	●	●		●	●	●		●				●		●		●			
	Atmospheric Transport Model	●	●					●	●			●				●	●				●	●	●	●	●	●	●		●		●			●	●	●	●		●		●	●		
	Drift Transport Cooling Tower [b]							●								●				●	●					●	●		●		●	●					●		●	●	●	●		
	TRC Cooling System [b]									●	●									●	●	●				●	●		●	●	●	●	●	●	●	●	●		●	●	●	●		
	Texas Episodic Model	●	●	●	●	●																●		●	●	●	●	●	●		●	●					●			●	●	●		
	Texas Climatological Model	●	●	●	●	●																●		●	●	●	●	●	●		●	●					●		●		●	●		
	NUMERICALLY INTEGRATED																																											
	IBMAQ 1&2	●	●																			●		●	●	●	●		●	●		●						●		●	●	●		
	INTERA [b]	●	●	●	●																●	●		●	●	●	●		●	●	●	●			●	●		●		●	●	●		
	ADPIC	●	●	●																	●	●			●	●	●		●	●	●	●			●	●		●		●	●	●		
	ACOSP					●																		●	●		●		●		●	●		●				●		●	●	●		
	LIRAQ I [a]	●				●																●		●	●			●	●		●	●	●	●	●	●		●		●	●	●	●	
	LIRAQ II [a]	●		●	●	●	●															●		●	●			●	●		●	●	●	●	●	●		●		●	●	●		
	Reactive Plume Model	●		●															●		●	●			●	●	●		●	●	●	●		●	●	●		●		●		●	●	

continued ....

Table 5-3. Air Quality Models and Their Relevance to Specific Problems (Continued)

		PROBLEM CHARACTERISTICS																																										
		RESIDUAL																			SOURCE						RECEPTOR				TERRAIN						TIME				SCALE			
	MODEL TYPE MODEL DESIGNATION	SO$_2$	Suspended Particulates	NO$_x$	HC$_x$	CO	Oxidants	Toxic Metals	Nutrients or Salts	Water Vapor	Sensible Heat	Radioactivity	Pesticides	Aeroallergens	Fugitive Dust	Surface Deposition (dry)	Surface Deposition (wet)	Acid Rain Deposition	Sulfates	Cooling Systems	Single Point Source	Multiple point sources	Line Source [a]	Area Sources	Ground-Level Discharge	Elevated Discharge	Point Receptor	Area Receptor	Ground-Level Receptor	Elevated Receptor	Smooth or Gently Rolling	Rough Urban	Shore or Coastal Area	Valley or Basin	Hilly or Mountainous	Forest	Steady-State	Dynamic	Long-Term	Short-Term	Up to a Few Km	Few Km to 50 Km or so	50 Km to 200 Km or so	Greater than 200 Km
CONSERVATION OF MASS	. NUMERICALLY INTEGRATED																																											
	Chemically Reactive Power Plant Plume Model			●			●														●				●	●		●	●	●	●				●	●		●		●	●	●		
	IMPACT	●	●	●	●		●												●		●	●		●	●	●		●	●	●		●			●	●		●		●	●	●		
	STIFF 3 [b]									●	●									●	●	●	●			●	●		●		●	●		●	●	●		●		●	●	●		
	Westinghouse C.T. [b,c,d]							●								●				●	●	●	●			●	●		●		●	●	●	●	●	●		●		●	●	●		
	REM 2 [e]			●	●	●	●															●		●	●			●	●	●	●	●	●	●				●		●		●		
	DIFKIN [a]			●	●		●															●		●	●			●	●	●	●	●	●	●				●		●	●	●		
	CEM	●	●	●		●																		●	●	●		●	●	●		●						●		●	●	●		
	SAI (1978 Version) [a] (Urban Air Shed Photochemical)	●	●	●	●	●	●															●	●	●	●	●		●	●	●	●	●	●	●	●			●		●	●	●	●	
	NEXUS	●	●	●	●	●	●														●	●		●	●	●		●	●	●	●	●			●	●		●		●	●	●		
	. PROPORTIONAL																																											
	Rollback / Rollforward Appendix J	●	●	●	●	●	●																									●					●		●	●		●		
	. STATISTICAL																																											
	Croke - Roberts	●	●	●	●	●		●								●	●				●	●		●	●	●	●		●	●	●	●	●	●	●	●	●		●	●	●	●		
	Repro Model			●			●																								●	●	●	●	●	●				●	●	●		

[a] frequently used for mobile sources [b] proprietary [c] C.T denotes cooling tower [d] model used for cooling tower droplet deposition (drift deposition)

[e] Air Quality Submodel of the Transportation and Air Shed Simulation Model

Procedure for Selecting an Appropriate Air Quality Model

The procedure for selecting an air quality model is directly tied to steps 4 and 5 in the section on setting up the natural systems analysis in chapter 2. Given that the natural systems analysis required in a given REQM context has been specified in terms of the relevant characteristics of the air quality problem or problems of concern, the analyst would then follow the procedure contained herein. The procedure indicates the questions which must be asked and the activities undertaken before an appropriate model can be selected, given operational constraints. Further, the procedure is the vehicle which operationally integrates the various sections of this chapter. Figure 5-19 is a flow chart of the steps in selecting an appropriate air quality model. Note that the flow chart is slightly different from the flow chart of the NSM selection process contained in figure 2-6 of chapter 2.

Given that the required natural systems analysis has been specified, the procedure begins with a search of the problem table. If one or more candidate models is or are identified as operational, the analyst then goes to the summary tables in appendix A to tabulate the relevant information for each of the candidate operational models. Table 5-4 is the model summary table prepared for the Gaussian Evaluation Model developed by Fabrick, Sklarew, and Wilson of Science Applications Incorporated, Westlake Village, California. The descriptions of the characteristics shown on this table which pertain to all NSMs are discussed in chapter 2. Additional points relating to these characteristics with respect to air quality models, and descriptions of characteristics applicable solely to air quality models, are contained in the next section.

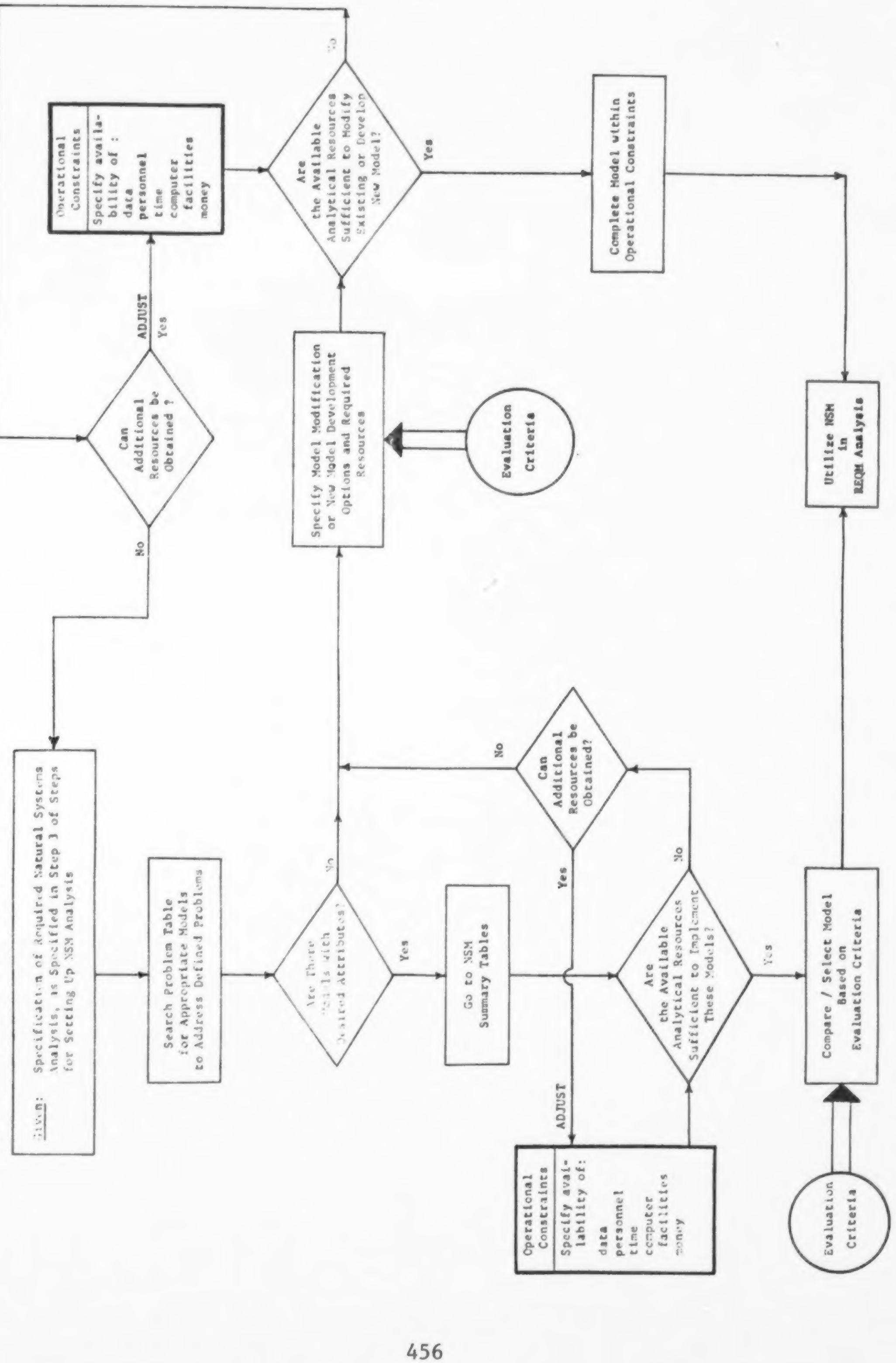

Given: Specification of Required Natural Systems Analysis, as Specified in Step 3 of Steps for Setting Up NSM Analysis
Search Problem Table for Appropriate Models to Address Defined Problems
Are There Models with Desired Attributes?
Yes
No
Go to NSM Summary Tables
Are the Available Analytical Resources Sufficient to Implement These Models?
Yes
No
Can Additional Resources be Obtained?
Yes
ADJUST
No
Operational Constraints
Specify availability of: data personnel time computer facilities money
Compare / Select Model Based on Evaluation Criteria
Evaluation Criteria
Utilize NSM in REQM Analysis
Specify Model Modification or New Model Development Options and Required Resources
Evaluation Criteria
Are the Available Analytical Resources Sufficient to Modify Existing or Develop New Model?
Yes
No
Complete Model within Operational Constraints
Can Additional Resources be Obtained ?
No
Yes
ADJUST
Operational Constraints
Specify availability of : data personnel time computer facilities money

Figure 5-14. Procedure for Selecting an Air Quality Model

Table 5-4. Summary of Gaussian Evaluation Model (GEM)

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain, except where there are severe localized distortions to dominant area wind flows
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) decay
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly ambient concentrations, averaging periods up to 24 hours
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) meso; (3) discretization: (a) one layer; (b) up to 100 user-specified receptor locations; (4) resolution: (a) inputs: residuals discharges, meteorological data as point data; (b) outputs: ambient point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) multiple point source residual discharges; (b) stack parameters: stack height, temperature, stack gas flow rate; (c) meteorological data vary somewhat with calculational options chosen (see model accuracy): some combination of hourly stability class, hourly horizontal standard deviation of wind direction, hourly horizontal wind direction change with height, hourly wind speed, mixing height; (d) decay rates of residuals; (e) surface roughness parameter; (f) ambient air quality concentrations; (g) receptor co-ordinates; (2) verification: (a) independent set of meteorological data; (b) independent set of ambient concentrations
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/168 or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: final report and user's guide available which describe: (a) theory; (b) subroutines and model options; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer: (b) research assistant; (4) model user qualities: (a) mathematical abilities through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model output or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration; (2) values given at: (a) specific points; (b) hourly averages, or time period averages not to exceed 24 hrs.: (3) format. (a) tabular printout
Costs	(1) model acquisition: (a) model user's guide, final report and listing available at no charge; (2) model set-up: (a) program set-up and debug could be accomplished within a few man-weeks; (3) data preparation: (a) data acquisition and preparation could be obtained within a few man-days; (b) keypunching of data could be accomplished within a few man-days; (4) actual computation: (a) typically $20 or so; (5) output analysis: (a) validation and verification could each be performed within a man-week or so
Model Accuracy and Sensitivity	(1) representativeness to prototype system: as a Gaussian point source model intended for application in complex terrain, GEM provides several options for calculation of key parameters, generally to allow for realism or conservatism in estimates: (a) three options for plume rise formula, or plume rise may be user-specified; (b) mixing height can be assumed to remain horizontal or to be displaced upward over elevated terrain; (c) four variations for treatment of elevated plume position in relation to elevated terrain; (d) three variations for treating effect of complex terrain upon horizontal diffusion parameter, or value may be user-specified; (e) three options for including effects of terrain surface roughness upon vertical diffusion parameter, or value may be user-specified; (f) two options for treatment of limited mixing condition; (2) model accuracy: (a) although model developers made considerable attempts to test their model over complex mountainous terrain and coastal terrain, it is clear that much more validation is needed, in part because the model has so many combinations of options; (b) model developers concluded that the model seemed to work somewhat better in the inland mountainous rather than the coastal terrain, that vastly different results were obtained depending upon the combination of model options chosen, and that it appears that (with good judgment in selection of options) the Gaussian formulation can predict the hourly maximum concentration within a factor of two and the downwind distance within a factor of two during unstable atmospheric conditions; (3) model sensitivity: although this topic was not formally studied, it is clear that: (a) ambient concentrations are quite sensitive to the different options for treating plume position in comparison to elevated terrain and to the treatments selected for calculating horizontal and vertical diffusion parameters; (b) model is insensitive to option selected for limited mixing
Other Comments	(1) model limitations/restrictions: (a) model not suitable where there are large variations in wind direction (such as within complex canyon and in coastal regions); (b) model not intended for "long-term" annual average applications; (2) special features: (a) ability to accept user-specified data is important feature; GEM model could incorporate empirically derived plume parameters from tracer or plume photography studies; (b) model developers have attempted to include best available options to account for terrain elevation and roughness effects; (3) application has been applied to a smelter in Utah and power plant in California, both in complex terrain

Note: Also included in Appendix A as table 5A-14.

Next, the available analytical resources to utilize the identified models are compared with the resources required. If several models can be applied within the operational constraints, then a model is selected on the basis of the evaluation criteria discussed in chapter 2. If only one model can be applied within the operational constraints, then that model would be chosen, unless it did not meet some evaluation criterion deemed critically important.

If none of the candidate operational models can be applied within the operational constraints, the logical first option is to attempt to increase the available analytical resources to the level required to apply at least one of the candidate operational models. If additional resources cannot be obtained, or if no operational models can be located in the problem table which are capable of addressing the problems of concern, the analyst has three choices. First, the literature can be searched to locate operational models--not included in the problem table--which would satisfy the requirements of the analysis. In order to choose among any additional models discovered--in relation to operational constraints and evaluation criteria--information comparable to that contained in the model summary tables in appendix A should be obtained for these models. Second, modifications could be made to an existing model to satisfy analytical specifications, given operational constraints and the evaluation criteria. Third, a new model could be developed from "scratch." The second and third choices are shown in the flow chart of the selection procedure; the step of obtaining the requisite information on other, possibly operational, models is not. The possibility will always exist that there are models described in the literature and heretofore passed over which, when investigated, could be suitable in a given context. If none of the above options can be accomplished due to operational constraints, the evaluation criteria, or lack of knowledge, then the required air quality analysis, that is, the questions to be answered, must be respecified and the procedure repeated.

Developing a new model from scratch entails basic theoretical mathematical formulation, debugging after set-up, sensitivity testing, calibration, and verification. These together represent a level of effort considerably above that involved in applying an existing operational model. Model development requires certain specialized technical skills and substantial resources. It should be undertaken in an REQM analysis only after very careful consideration.

Finally, the procedure described above should not be viewed only in terms of the information presented in this chapter and its appendices. The activities and questions identified are relevant for selecting an air quality model under any analytical conditions.

Characteristics Used to Summarize Air Quality Models

Table 5-4 illustrated the way in which operational air quality models are summarized in the tables comprising appendix A. Thirteen characteristics are shown for which information on operational air quality models is provided. Seven of these characteristics--input data requirements, computation status, ease of application and manpower needs, output and output format, costs, linkages to other models, and model accuracy and sensitivity--were described in chapter 2, because they are defined similarly regardless of the type of NSM. The other six characteristics are discussed here. Also, some specific comments are made about the input data requirements in relation to air quality models.

Terrain Characteristics

Type of terrain in an important consideration because different air quality models were developed with parameters applicable to specific types of terrain. As a result, a model may be less accurate for, or may require modification in its application to, types of terrain other than that or those for which it was developed. Six somewhat overlapping terrain and land use characteristics have been identified to determine applicability: (1) smooth or gently rolling; (2) shore or coastal area; (3) valley or basin; (4) mountain; (5) "rough" urban area; and (6) forest. Obviously, combinations of these types exist; often such combinations are important in practical problems.

Physical Processes

All air quality NSMs treat one or more of the following four physical processes in one form or another, either explicitly or implicitly: (1) transport (advection); (2) diffusion; (3) dry deposition; and (4) wet deposition.

Chemical Processes

Two types of chemical processes are identified: (1) decay; and (2) photochemical oxidation.

Mathematical Properties

Two categories of mathematical characteristics are delineated: (1) type of mathematical relationship; and (2) solution methodology. "Type of mathematical relationship" differentiates between deterministic and stochastic models. In practice, all air quality NSMs are deterministic in the sense that an equation is used to indicate a cause and effect relationship between air quality concentration and independent variables for a specified set of conditions. However, many deterministic models have statistical components, representing stochastic events, imbedded within them.[26] For example, the diffusion terms in the conservation of mass equation represent a stochastic phenomenon, namely the stochastic turbulent fluctuations which cause residuals to diffuse. The diffusion parameters in the Gaussian equation similarly represent a stochastic phenomenon. Both may be statistically derived, based on empirical measurements.

Three classes of solution methodologies are identified: (1) analytically integrated (Gaussian); (2) numerically integrated; and (3) statistical.

Time Properties

Time properties identified are: (1) time variability of inputs; and (2) time period of outputs. Time properties are important in the choice of an air quality model, choice of data input to the model, and to interpretations of outputs from the model.

Time variability of inputs is expressed as "steady state," "quasi-steady state," or "dynamic," and refers to the extent that inputs to the model are varied from one time unit to the next, and succeeding time units comprising the period of analysis, for example, from hour to hour during a 24 hour period. With a "steady state" model, the model inputs--residuals discharges and meteorologic conditions such as wind speed, wind direction, atmospheric stability--do not vary over the time period of analysis. With a "quasi-steady state" model, some inputs are varied from one time unit to another while other inputs are held constant. For example, residuals discharge rates may be held constant while meteorologic conditions vary, or vice versa. With "dynamic" models, all inputs are varied from one time unit to the next during the time period of analysis. In practice, both quasi-steady state and dynamic models are usually assumed to be "piecewise constant," such that variables may vary from hour to hour but are assumed to be constant during a given hour.

The time period of outputs refers to the "averaging time" for which the outputs of estimated concentrations are desired. Different models yield average values for different time periods, while various time periods are used for different air quality management problems. Time periods of outputs range from a single hour or daily time period or a combination of daily time periods which form an air quality "episode" of adverse air quality lasting for a few days, to seasonal and annual time periods. For the longer time periods the models used are generally of a steady state or quasi-steady state type, while for the shorter time period steady state, quasi-steady state, and dynamic Gaussian models and dynamic numerically integrated models have been used.

Space Properties

Space properties of air quality models are: (1) dimensionality, expressed as one, two, or three dimensions; (2) scale, expressed as a range of distance over which a model is intended for application; (3) discretization, expressed as a dimensionless number; and (4) spatial resolution of inputs and outputs, expressed as point, line, or area dimensions.

With respect to the first, the number of dimensions which a model represents reflects the number of dimensions of residuals concentrations and ambient environmental quality which can be estimated. For example, a three-dimensional model enables simultaneous estimates to be made of residuals concentrations in the vertical and horizontal dimensions. A two-dimensional model assumes homogeneity of ambient concentration in either the vertical or one of the horizontal dimensions. As the number of dimensions increases, the complexity of a model and related data requirements, computer storage requirements, and computation costs also increase.

With respect to the spatial scale of application, particular air quality NSMs are intended for application over particular ranges of distances. Some models are appropriate for examining localized impacts in the vicinity of local discharge sources, for example, highways or factories, up to a few kilometers downwind. Such models are referred to as "microscale" models. Models which are appropriate for analyzing entire urban areas, for example, up to about thirty or fifty kilometers in length and width, or for analyzing small regions, for example, up to 200 kilometers or so in length, are referred to as "mesoscale" models. These mesoscale models enable the analysis of the contributions to air quality concentrations in one urban area from residuals discharges in another. Additionally, models are now being developed to assess ambient air quality impacts of large point sources or complete urban areas at "macroscale" distances of several hundred or one or two thousand kilometers downwind.

Discretization refers to the degree of spatial aggregation used for model inputs and outputs. Some air quality models treat the vertical dimension of the atmosphere as being comprised of one layer, frequently with homogeneous characteristics; other models represent the vertical dimension with multiple layers and allow characteristics to vary from layer to layer. Similarly, many models require the use of horizontal grid areas of varying numbers and sizes in the specification of model inputs and outputs. The level of discretization is an important factor in computer storage and computational requirements.

Closely related to discretization is model "resolution." Resolution refers to whether the inputs of the model are treated as point, area, or line sources and whether the outputs are treated as point or area (grid) average concentrations. If the output concentrations are area-averaged, it is important that the proper grid discretization be used so that important localized "hot spots" are not smoothed out. The problem of appropriate model resolution is dependent upon the particular residual and its discharge sources, the problem being addressed, the locations of receptors, and the spatial scale of the question being investigated. For example, concentrations of photochemical products which react rather slowly and become significant at distances several kilometers away from major discharges do not require a high degree of resolution. On the other hand, if a discharge can be expected to cause its largest impact within a few kilometers of the discharge location, greater resolution is required.

Input Data Requirements

Model input requirements have been divided into: (1) initial setup and calibration; and (2) verification. For both of these categories, four types of input data are always required: residuals discharge data, meteorologic data, ambient air quality concentration data, and location coordinates for sources and receptors. For some models two additional types of data are required: stack parameters for models which calculate plume rise as a subroutine and reaction rates or "decay" factors for models which explicitly treat chemical processes. Stack parameters include height and diameter of stack, exit temperature of gas, and the exit velocity of air flow at the top of the stack. Often the latter two parameters are specified differently for "short-term" as opposed to "long-term" time periods.

Residuals discharges are required for point, area, and line sources and are expressed as units of discharge per time unit. Frequently residuals discharge data are collected and summaried in English units, while diffusion models always calculate ambient concentrations in metric units. Thus care must be taken to provide the residuals discharge data in units specified by the computer program; some programs have "conversion factors" from English to metric units, while others do not.

Meteorologic data required may include wind speed and direction, mixing height, and atmospheric stability class. Some models require these data from multiple points within the region of interest, while other models operate with data from only a single point. Generally, hourly values of wind speed at one or more elevations, wind direction, and stability class are required. For elevated discharges it is desirable to have wind speed data representative of the stack height. For models which calculate "long-term" average concentrations, hourly data are often required in the form of a joint frequency of occurrence for sixteen wind directions, several stability classes, and several wind speed classes.[27] For "long-term" models, single average seasonal or annual average values of mixing heights may be used, while "short-term" models which require mixing heights generally require hourly values.

One set of data on ambient air quality concentrations is required to calibrate a model, and another--independent--set is required to verify the model. The amount of data required for calibration and verification varies substantially as a function of the natural system being modeled, the time period of analysis, and the question(s) being answered. Detailed assessments of spatial and temporal variations in ambient air quality can require huge amounts of data. In general, most REQM applications would require measured data on ambient concentrations at a number of points.

Concluding Comment - Model Selection

The foregoing has discussed the requisite steps for choosing an air quality NSM for a given application. The procedure described is applicable regardless of the context. The characteristics chosen to summarize the operational models contained in appendix A are useful for describing all air quality models.

Germane to any discussion of model selection is identification of problems which relate to model application. An understanding of these problems enables more intelligent use to be made of the available materials on air quality models, included herein and elsewhere, for selecting a model appropriate for a given context. The last section in chapter 2 describes major problems relating to applications of natural systems models. These problems are generally relevant for all categories of NSMs, and should be reviewed before embarking on model selection.

CONCLUDING COMMENTS

Although operational air quality models have been developed, some of which have had wide application, three problems with respect to such models and air quality problems merit emphasis. The first relates to procedures for applying air quality models. In connection with calibrating and verifying air quality models, statements have often been made that a model performs "well" if the ambient concentration estimated within the model is within a factor of 1 or 2 of the measured concentration, for short-term analyses. Assuming that the measured concentration is a reasonably accurate measure of the "true" concentration, the often substantial differences between estimated values and measured values need to be explained. One possible explanation is the typical procedure, in developing input data for short-run air quality models, of assuming constant discharges of gaseous residuals, at the same time that the meteorologic conditions are varied from time unit to time unit over the period of analysis, for example, each hour over a four or five day episodic period. Given the highly stochastic nature of gaseous residuals discharges from many activities, more consideration should be given to the consistency of the input data on residuals discharges and meteorologic conditions in the analysis of air quality management problems.

A second problem involves flows of airborne residuals across boundaries of regions and across boundaries of existing political jurisdictions. Such cross-boundary flows are of such magnitude that for some, or many, regions it will be impossible to meet ambient air quality standards by installing physical measures solely at dischargers within a given region. Cross-boundary flows involve both short-range transport, such as within major metropolitan areas, for example, New York, as discussed in Rubino, et al. (1976), and long-range transport, such as from the Midwest to the New York region, as discussed, for example, in Wolff, et al. (1977). The five-year (1972-1976) OECD program to measure inter-country transport of sulphur compounds reflected similar concern for long-range transport (OECD, 1977).

The third problem, closely related to the second, involves the impacts of airborne residuals on ambient water quality. For example, awareness of the existence and potential impacts of acid precipitation has increased substantially in recent years. The problem is complicated by the vaired constituents composing acid rain, for example, as discussed by Liljestrand and

Morgan (1978) for the Pasadena, California area. As evidence has accumulated from various studies, it is now recognized that a wide range of residuals can be transported through the atmosphere and be discharged into water bodies with resulting adverse effects on ambient water quality. Included are nitrogen and phosphorus, as discussed, for example, by Nicholls and Cox (1978), and PCBs, as discussed, for example, by the Great Lakes Basin Commission (1976).

NOTES

[1] To a large extent, boundaries for analyzing atmospheric systems in the United States have been specified under the mandated planning requirements of the Clean Air Act. These areas have been designated "air quality control regions" (ACQRs). Many of them correspond to Standard Metropolitan Statistical Areas.

[2] The transport of residuals long distances from the region of generation to other regions is termed "long-range transport."

[3] An operational NSM as defined herein has two attributes. The first is that it has been successfully applied to and verified for at least one application and that it can be used to model another different, but roughly similar, system without extensive internal modification. The second is that sufficient written documentation must be available about the model to enable a user to apply the model in a location other than that for which it was verified.

[4] By mid-1981, some models for fugitive dust, regional haze, and plume visibility were probably operational as defined herein. This is also probably the case for at least a few long-range transport models. (See Michael, 1980).

[5] The term precursor is used to describe all substances that would participate in the photochemical reactions producing oxidants.

[6] Epidemiologic studies are studies which seek to analyze the effects of diseases on populations. Epidemiologic studies have the advantage of focusing on real populations in their normal settings. However, the health indexes they use are relatively crude, and they are typically unable to isolate the effect of one environmental factor from all of those acting on a given population.

[7] Leaf chlorosis is a diseased condition in green plants marked by yellowing or branching.

[8] Council on Environmental Quality (1978), p. 4.

[9] Of course chemical composition, as well as particle size, is relevant to impacts on human health.

[10] A number of recently developed air quality models have been designed specifically to deal with "complex terrains," e.g., valleys, hills, mountains.

[11] It merits emphasis to indicate that it is very difficult to obtain accurate information on meteorologic conditions and practically impossible on residuals discharge conditions for averaging periods of less than 24 hours.

[12] See table 2-1 in chapter 2.

[13] The phenomenon in which heat is absorbed by urban areas during the daytime and released at night, tending to prevent very stable conditions from occurring, is known as the heat island effect.

[14] A hydrometeor is defined as a product of the condensation of atmospheric water vapor, e.g., rain droplets, hail, fog, and snowflakes.

[15] It should be noted that processes which break down ozone occur simultaneously with processes which form ozone. Ozone concentration only becomes a problem when the latter exceeds the former over time.

[16] A possible fifth procedure is known as the "modified" Pasquill-Turner.

[17] It has become common practice to add a seventh category, very stable, although this was not proposed by Pasquill or Turner.

[18] In many areas, the National Climatic Center has summarized meteorologic data into the stability category format required for input into Gaussian models. Of course, as always, whenever data from one location are being applied to other locations, care must be taken that the data used are "representative" of the location being evaluated. For example, frequently cities may be located in valleys, while the meteorologic data are from airports on plateaus. Judgement or additional "on site" measurements may be required in order to adjust successfully the wind speeds and wind directions on the plateau to be representative of those in the valley.

[19] It should be noted that the Nuclear Regulatory Commission (1972) has adopted a quantitative scheme for classifying intervals of temperature gradient into the Pasquill-Turner stability categories.

[20] For analyzing "hot spot" problems--that is, receptor locations having very high ambient concentrations--the analysis starts at the receptor point and the trajectory is run backwards in time to determine the contributions to ambient concentrations at the receptor point from the various sources.

[21] For a summary of the DIFKIN model see table 5A-29 in Appendix A.

[22] Note, figure 5-7 illustrates how NO, NO_2, and O_3 concentrations vary over time.

[23] One recent example of the use of another statistical method is the development of a conditional Markovian model by Carlson and Umble (1979) for estimating the probability that ambient concentrations in a region will reach a specified level within a given time period.

[24] For additional discussions of the use of the statistical approach see Caporaletti, et al. (1977), Kinosian and Paskind (1973), Myrabo, et al. (1977), Trijonis (1978), Marians and Tiao (1975).

[25] Not all rollback models are so limited; some include both hydrocarbons and NO_x. For discussions of modified rollback models see Chang and Weinstock (1975), Nevers and Morris (1975), and Horie (1974).

[26] There are "statistical" air quality models, such as extreme value theory, which are not natural systems models in terms of the definition used herein, i.e., NSMs translate spatial and temporal patterns of residuals discharges into spatial and temporal patterns of ambient concentrations.

[27] When airport meteorologic records are used, records of hourly data frequently are not available.

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Appendix A:.

SUMMARY TABLES OF AIR QUALITY MODELS

Table 5A-1. Summary of Gifford-Hanna Model

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none (in nonreactive model version)
Mathematical Properties	(1) type of relationship: (a) deterministic
Time Properties	(1) time variability of inputs: (a) steady-state, (b) quasi-steady-state; (c) dynamic; (2) time period of outputs: (a) long-term: seasonal, annual average; (b) short-term: daily, few hours or less
Space Properties	(1) dimensionality: (a) three; (2) discretization: (a) user-specified number of area grids and grid size for sources and receptors; (3) resolution: (a) inputs: residuals discharges as grid area sources, single point meteorological data; (b) outputs: grid area concentrations
Input Data Requirements	(1) initial set-up and validation: (a) area residuals discharge sources; (b) point meteorological data: hourly wind speed and direction, stability class; (c) several ambient air concentration measurements; (2) verification: (a) residuals discharges (see above); (b) meteorological data (see above); (c) ambient air concentration measurements
Computation Status	(1) model status: (a) uncoded; (2) equipment needed: (a) hand calculator
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: (a) no formal manual exists, but information available from author articles, authors, and other sources (see annotated bibliography); (3) expertise required: (a) no specific job description required; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs, or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentrations: SO_2, suspended particulates, NO_x, HC_x, CO; (2) values given at: (a) grid areas, (b) ground-level
Costs	(1) actual computation: (a) dependent upon size of urban area, time variability, and time period (i.e., long-term or short-term); initial hand calculations may require a few hours to a few days of man-time
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: single point meteorological data do not describe micrometeorological variations within city, nor "urban heat island" air circulations. (b) simplifying assumptions: ambient concentration can be universally estimated as a simple function of stability, wind speed, and residuals discharge rate; (2) model accuracy: (a) varies with different variations of model, but roughly comparable to more sophisticated models for suspended particulates; (b) a rather large range of error is apparent; (c) for sulfur dioxide it is particularly important to determine concentrations from large point sources by another model and add these concentrations to outputs from Gifford-Hanna model; (3) model sensitivity: (a) model sensitive to wind speed, rather insensitive to atmospheric stability
Other Comments	(1) model limitations/restrictions: (a) basic model designed for area sources only, i.e., model best suited where there are no large point or line sources or in combination with point or line source models; (2) special features: (a) model does not require use of computer; (b) a few variations of basic model are in use; (c) model can be used for both long-term and short-term applications; (d) "pure" natural systems model; (3) application experience: (a) model has been applied and tested in several cities including Chicago, Los Angeles, Nashville, and San Francisco

Table 5A-2. Summary of Gifford-Hanna Photochemical Model

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) photochemical reaction rates and equations included for NO, NO_2, reactive hydrocarbons; (2) ozone assumed to be proportional to the ratio of NO_2 to NO
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) steady-state algebraic solution; model could also be solved with a dynamic, numerical integration--such as Runge-Kutta--though not undertaken by author
Time Properties	(1) time variability of inputs: (a) quasi-steady-state; (2) time period of outputs: (a) short-term: hourly concentration
Space Properties	(1) dimensionality: (a) uniform, average concentration in x, y, z for whole urban area; (2) spatial scale of application: (a) meso; (3) resolution: (a) inputs: discharge sources and wind speeds are averaged for the whole urban area; (b) outputs: average concentration for whole urban area
Input Data Requirements	(1) initial set-up and validation: (a) area discharge rate for reactive hydrocarbons; (b) hourly average area wind speed; (c) ambient concentration measurements of NO_2 and NO at 6 a.m. or area discharge rates of NO_2 and NO; (d) ambient hourly measured concentrations for NO, NO_2, reactive hydrocarbons, O_3 to calibrate model; (2) verification: same as for calibration
Computation Status	(1) model status: uncoded
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: (a) no formal user's manual exists, only complex technical published article available, inexperienced user would need much guidance from author or experienced modeler; (3) expertise required: (a) no specific job description required; (4) model user qualities: (a) mathematical ability through advanced calculus; (b) knowledge of specialized model solution techniques; (c) specialized knowledge of model assumptions and principles, including photochemistry and understanding of model limitations; (d) prior experience with this kind of modeling desirable, otherwise access to consultations mandatory
Output and Output Format	(1) type of output: (a) ambient concentrations: HC_x, oxidants; (2) values given at: average for urban area
Costs	(1) for experienced users, model typically requires about one man-week to gather air quality data and perform hand calculations, not including residuals discharge data compilation; (2) calibration and verification would each probably require a few more man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description and simplifying assumptions: "steady-state" solution for photochemistry is simplification, uniform "box model" for urban area is simplification of transport/diffusion process, homogeneous residuals discharges; (2) model accuracy: (a) based upon limited field studies in Denver and Los Angeles, model highly underpredicts ozone concentrations, while predictions for other residuals are inconclusive; (3) model sensitivity: (a) ozone concentration calculation wholly dependent upon calculated ratio of NO_2/NO
Other Comments	(1) model limitations/restrictions: (a) model provides hourly average ambient concentration estimates for the whole urban area, spatial variations within region are not predicted; (2) special features: (a) model does not require the use of a computer (though this does not mean model application is simple); (b) "pure" natural systems model; (3) application experience: on the basis of published studies, model use has been rather limited

Table 5A-3. Summary of the Air Quality Display Model (AQDM)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: seasonal, annual average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) up to 14 x 14 grid and grid size is user-specified; (c) up to 225 grid receptor and up to 12 additional receptor points are user-specified; (4) resolution: (a) inputs: residuals discharge data as point or area sources, single point meteorological data; (b) outputs: point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point and area residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data: joint frequency of wind speed (six classes), wind direction (sixteen directions), and stability class (five classes), annual or seasonal mixing height; (d) several ambient air concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharge data; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 360/40 or equivalent; (b) a maximum of 300,000 bytes; (c) program language: FORTRAN IV (level G)
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) model documentation available: (a) theory; (b) subroutines; (c) data deck; (d) format; (e) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration of SO_2 and suspended particulates; (2) values given at: (a) grid locations; (b) other user-selected points; (c) ground-level; (3) format: (a) tabular printout; (b) card deck for use with CALCOMP or SYMAP plot programs; (4) special features: (a) statistical output subroutine; (b) receptor contribution analysis; (c) calibration subroutine
Costs	(1) model acquisition: (a) public, "as is" model and user document cost about $5; (2) model set-up: (a) program set-up and keypunch: 8 man-days; (b) test case and de-bug: 10 man-days; (3) data preparation: (a) analysis and reduction: 3 man-days; (b) keypunched or recorded: 2 man-days; (4) actual computation: dependent on problem and number of sources and receptors, upper limit is less than $25 run; (5) output analysis: (a) analysis of results: varies with problem, but routine validation/verification can each be done in 5 man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: fixed-point meteorological data do not describe micrometeorological variations within city nor "urban heat island" air circulations; (b) simplifying assumptions: Gaussian diffusion, homogenous diffusion; (2) model accuracy: (a) model tends to overestimate; (3) model sensitivity: (a) known to be sensitive to effective stack height, wind speed, and stability
Other Comments	(1) model limitations/restrictions: (a) limited to SO_2 and suspended particulates; (b) designed for annual average and seasonal applications; (2) special features: (a) model is "conservative"; (b) has popular special output features (previously noted); (c) AQDM has been incorporated into the EPA Implementation Planning Program (IPP); (3) application experience: (a) model is one of the most widely used and best tested for state implementation plans

Table 5A-4. Summary of Climatological Display Model (CDM)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion; (2) dry deposition can be accounted for in the user-specification of a "half-life"
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian model with some numerical approximations
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: seasonal, annual average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer: (b) up to 50 x 50 grid areas and grid size is user-specified; (c) user-specified number of receptor points at user-specified locations; (4) resolution: (a) inputs: residuals discharge inputs as point or area sources, single point source meteorological data; (b) outputs: point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point and area residuals discharges; (b) stack parameters: height, diameter, temperature, exit-velocity; (c) meteorological data: joint frequency of wind speed (six classes), wind direction (sixteen directions) and stability class (six classes), annual average or seasonal mixing height; (d) several ambient concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) for use in interactive mode a terminal is required; (b) for use in batch mode a digital computer is required; (3) computer characteristics: (a) IBM 360 or IBM 370 or equivalent; (b) program language: FORTRAN IV (level G)
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user guide available with: (a) theory; (b) subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and assumptions and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration of SO_2 and suspended particulates; (2) values given at: (a) user-specified points; (b) ground-level; (3) special features: (a) calibration subroutine; (b) receptor contribution analysis;* (c) statistical output subroutine*
Costs	(1) model acquisition: (a) public, "as is" model listing and user document available free or at a nominal cost; (2) model set-up: (a) program set-up and keypunch: 8 man-days (estimated); (b) test case and de-bug: 10 man-days (estimated); (3) data preparation: (a) analysis and reduction: 3 man-days (estimated); (b) keypunched or recorded: 2 man-days (estimated); (4) actual computation: dependent upon problem and number of sources and receptors, generally less than $20/run; (5) output analysis: (a) graphics and data plotting costs not specified; (b) analysis of results varies with problem, but routine validation/verification can each be done in 5 man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: fixed point meteorological data do not describe micrometeorological variations within city nor "urban heat island" air circulations, representation of wind speed as a "power law" function of height is an improvement upon AQDM, use of Briggs plume rise formula also is an improvement; (b) simplifying assumptions: Gaussian diffusion, homogenous diffusion; (2) model accuracy: (a) comparatively small absolute errors; (b) comparatively low standard errors; (3) model sensitivity: (a) known to be sensitive to effective stack height, wind speed, stability
Other Comments	(1) model limitations and restrictions: (a) intended for SO_2 and suspended particulates; (2) special features: (a) designed to accept meteorological (airport) data summaries from National Climatic Center Star Program; (b) has modeling improvements in comparison to earlier AQDM, as noted above; (c) interactive model available; (d) part of EPA UNAMAP series; (e) new version has popular output features noted above; (3) application experience: (a) model is one of most widely used and best tested for state implementation plans

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*This feature is found in updated version of model with CDMQC subroutines as published in Addendum to User's Guide for Climatological Dispersion Model, EPA-450/3-77-015, May 1977.

Table 5A-5. Summary of Air Quality Submodel of the Transportation and Air Shed Simulation Model

Characteristic	Summary Data
Terrain Characteristics	(1) intended for use in urban area located in flat or rolling terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: annual average concentrations; (b) short-term: concentrations computed from annual average using Larsen model
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) meso; (3) discretization: (a) one layer; (b) up to 150 area grid sources; (c) up to 150 receptor locations consisting of area source centroids and other receptor points; (4) resolution: (a) equal to grid area size
Input Data Requirements	(1) initial set-up and validation: (a) point sources: TASAQD subroutine requires residuals discharge rates, stack height, stack diameter, stack temperature, gas exit velocity; (b) area sources: subroutine EMIT requires numerous data inputs relating to spatial distribution, vehicle miles traveled, residuals discharge (emission) factors for different transportation types, vehicle speed information and correction factors, grid residuals discharge inventory for small stationary sources; (c) receptor co-ordinates for point and area sources; (d) meteorological data: EMIT subroutine requires mean annual average wind speed for each wind direction, annual frequency of each wind direction; TASAQD subroutine requires single stability class, annual mixing height, annual joint frequency of occurrence of 16 wind directions and 3 (mean) wind speeds; (e) ambient air concentration measurements for calibration; (2) verification: (a) independent set of meteorological data (see above); (b) independent set of ambient air concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/145 or IBM 370/165; (b) 120,000 to 160,000 bytes typically required, depending upon program subroutine used; (c) program language: FORTRAN
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available containing: (a) theory; (b) subroutines; (c) data deck formats; (d) separate publication contains application to Boston region; (2) expertise required: (a) computer programmer; (b) research assistant; (3) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration; (2) values given at: (a) specific points (b) annual average periods and "short term" periods; (3) format: (a) tabular printout; (b) optional SYMAP graphical output; (4) special features: (a) statistical output subroutine for short-term periods
Costs	(1) model acquisition: (a) model listing available along with user guide at nominal cost of a few dollars; (2) model set-up: (a) program set-up and de-bug could probably be accomplished within a few man-weeks, sample test case would have to be developed additionally; (3) data preparation: (a) data acquisition and preparation could be accomplished within several man-days; (b) keypunching of program and data onto card deck from model listing could be accomplished within a man-week or so; (4) actual computation: application of the two TASSIM air quality submodels to Boston region cost about $25 or so; (5) output analysis: validation and verification could each be performed in a man-week or so
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) model incorporates both mobile and stationary (point and area) sources; (b) simplifying assumptions: Gifford-Hanna simplified Gaussian model used for area sources (including mobile sources), single stability variation of Gaussian frequency-weighted model used for large point sources; (2) model accuracy: (a) additional testing needed, but in Boston model appeared to work fairly well for annual average suspended particulate concentration and not very well for sulfur dioxide and nitrogen dioxide concentrations; (3) model sensitivity: has not been published
Other Comments	(1) model limitations/restrictions: (a) TASSIM air quality submodel intended for multiple urban mobile and stationary sources; (b) applicability to NO_x (which is reactive) is questionable; (c) reprogramming of model required for application to cities other than Boston; (2) special features: (a) TASSIM air quality submodel is rather unique in that it treats mobile and stationary sources through the two respective models noted above; (b) TASSIM air quality submodel is part of a much larger TASSIM model; a second TASSIM submodel projects detailed spatial distributions of trips and vehicle mode; a third TASSIM submodel converts trip information to spatial distributions of vehicular residuals discharges; (3) in total the complete set of TASSIM submodels--including trip generation, residuals discharges, and air quality submodels--is quite complex and requires a large amount of reprogramming to remove specific formulations and data used for Boston; (4) application experience: results have been published for Boston and Los Angeles only

Table 5A-5. Summary of California Line Source Dispersion Model (CALINE 2)

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) mathematical: analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly concentrations
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro (very localized); (3) discretization: (a) one layer; (b) user-specified number and location of receptor points; (4) resolution: (a) inputs: residuals discharges as line sources (with "virtual" area source adjustment to account for initial mechanical turbulent diffusion), point meteorological data (hypothetical or actual); (b) outputs: ambient point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) traffic volume; (b) average vehicular discharge factor; (c) average elevation of highway section relative to surrounding terrain; (d) average highway width, including median; (e) meteorological data: hourly wind speed and wind direction relative to highway, hourly stability class; (f) ambient concentration measurements; (g) highway source coordinates; (h) receptor coordinates; (2) verification: (a) traffic volume; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) type of equipment needed: (a) digital computer for batch mode; (3) computer characteristics: (a) IBM 370/168; (b) typical run of 42 separate line source simulations with 36 receptor points required 11.5 CPU seconds; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available for: (a) batch mode: theory, subroutines, card deck format, test case; (b) interactive mode; (3) expertise needed: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model output or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration of NO_2, HC_x, CO; (2) values given at: (a) user-specified receptor points at user-specified heights; (3) format: (a) tabular printout
Costs	(1) model acquisition: (a) public, "as is" user's manual and program listing free of charge; (2) model set-up: (a) program set-up and keypunch: 10 man-days (estimated); (b) test case and de-bug: 5 man-days (estimated); (3) data preparation: very minimal, except for efforts required to develop vehicular traffic and discharge information; (4) actual computation: for typical computer run noted above, cost was $3; (5) output analysis: (a) negligible printout expense; (b) graphics/plotting routine must be set-up separately at nominal expense; (c) analysis of results: analysis and validation or verification could routinely be performed in five days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: highway is assumed to be an infinite line source, with different mathematical representations for the crosswind and parallel wind cases; (b) simplifying assumptions: to account for mechanical turbulence along highway, vehicular discharges are assumed to be evenly mixed through a volume of air dependent upon the highway width and twice the vehicle height, exhaust plume rise not explicitly included; (2) model accuracy: (a) for unstable or neutral conditions, field monitoring thus far indicates that there is a fairly high correlation between predicted and observed, but also a high standard error compared to the mean (a lot of scatter), accuracy during stable conditions is not determined; (3) model sensitivity: (a) based on fairly extensive sensitivity tests, model is known to be relatively sensitive to wind speed, stability class, and vehicular discharge, and relatively less sensitive to highway width and terrain elevation (over the range encountered)
Other Comments	(1) model restrictions/limitations: (a) model intended primarily for estimation of carbon monoxide only; (b) model intended for use at highway and off-highway receptors; (2) special features: (a) model available in batch or interactive modes; (b) model test results are presented in detail in user's manual; (c) model documentation is rather detailed and illustrated (though text is occasionally not easily comprehensible); (3) model experience: (a) model has been applied and tested in the Los Angeles area

Table 5A-7. Summary of EPA HIWAY Model

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerical integration of simple Gaussian equation
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: instantaneous or hourly concentrations
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro (very localized); (3) discretization: (a) one layer; (b) user-specified number and location of receptor points; (4) resolution: (a) inputs: residuals discharges as line sources, point meteorological data (hypothetical or actual); (b) outputs: ambient point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) in batch mode residuals discharges for vehicular line sources are input and in interactive mode residuals discharges are either input or they may be requested from program; (b) meteorological data: hourly wind speed; (c) ambient air concentration measurements; (d) highway source coordinates; (e) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) type of equipment needed: (a) digital computer for batch mode; (b) terminal for interactive mode; (3) computer characteristics: (a) type not specified, IBM 360 or equivalent would easily be sufficient; (b) magnetic tape characteristics: 9 track, 800 bits per inch, EBCDIC, odd parity; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available for: (a) batch mode: theory, subroutines, card deck format, test case; (b) interactive mode; (3) expertise required: (a) computer programmer; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration of NO_2, HC_y, CO; (2) values given at: (a) user-selected receptor points; (b) user-specified height; (3) format: (a) tabular printouts
Costs	(1) model acquisition: (a) public, "as is" user's manual and program listing free of charge; (2) model set-up: (a) program set-up and keypunch: 10 man-days (estimated); (b) test case and de-bug: 5 man-days (estimated); (3) data preparation: (a) very minimal, except for effort required to develop vehicular residuals discharge information; (4) actual computation: not specified, but very minimal cost; (5) output analysis: (a) negligible printout expense; (b) graphics/plotting routine must be set-up separately at nominal expense; (c) analysis of results: analysis and validation or verification could be routinely performed in five man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: treats highway as a finite, steady-state line source; (b) simplifying assumptions: with "grade-level" highway or "cut" highway, respectively, different initial plume dimensions assumed to compensate for mechanical turbulence generated by vehicles and highway, exhaust plume rise not explicitly included for "grade-level" highways; (2) model accuracy: (a) not discussed specifically by model developer, but one model user claims that off-highway estimates under stable atmospheric conditions and light winds are too high and that along-highway estimates are too high under all conditions;[*] (3) model sensitivity: (a) model known to be sensitive to wind speed and stability class, but not expected to be sensitive to mixing heights for model applications near highway
Other Comments	(1) model restrictions/limitations: (a) model intended only for estimation of ambient concentrations from vehicular discharges in the vicinity of highways, but not on the highway itself; (b) model used for residuals that can be considered to be "non-reactive" during the travel time of interest; (c) model requires additional validation; (2) special features: (a) model available as part of UNAMAP package of models; (b) model available in interactive mode; (c) model in batch mode is a "pure" natural systems model; (3) application experience: (a) limited experience to date suggests that HIWAY is better suited as a preliminary or screening tool than as a final decision tool

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[*] "General Motors Sulfate Dispersion Experiment: Assessment of the EPA HIWAY Model," Journal of the Air Pollution Control Association, January 1977, pp. 39-44.

Table 5A-8. Summary of Point, Area, Line Source Model (PAL)

Characteristic	Summary Data
Terrain Characteristics	(1) smooth
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated (Gaussian) with some numerical approximations
Time Properties	(1) time variability of inputs: (a) steady-state for any given hour of calculation, but "piecewise constant" from hour-to-hour; (2) time period of outputs: (a) short-term: hourly concentrations, up to 24 separate hours
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro, very localized; (3) discretization: (a) one layer; (b) up to thirty receptor points may be specified; (4) resolution: (a) inputs: residuals discharges as point, line, area sources, point meteorological data; (b) outputs: (a) point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point sources: residuals discharges, stack height, stack gas temperature, stack gas velocity, stack inside diameter, stack gas volume flow, stack co-ordinates, initial plume dimensions (if any); (b) area sources: residuals discharges, source height, source co-ordinates, area source length and width; (c) horizontal line sources: residuals discharges, source height, number of lanes (for highway), source endpoint co-ordinates, initial plume dimensions, total width of line source, width of highway median (if applicable), line source discharge for each lane (if multi-lane highway); (d) horizontal curved line sources: co-ordinates for endpoints and third point, source height, number of lanes, source width, width of highway median, initial plume dimensions, residuals discharges for each lane; (e) specialized line sources: residuals discharges, height of source endpoints, co-ordinates for endpoints, initial speed of vehicle at first endpoint, final speed of vehicles at second endpoint, initial plume dimensions; (f) specialized curved sources: residuals discharges, height of endpoints, co-ordinates of endpoints and third point, initial speed of vehicles at first endpoint, initial speed of vehicles at second endpoint, initial plume dimensions; (g) receptor co-ordinates and height; (h) meteorological data: wind direction, wind speed, stability class, mixing height, ambient air temperature; (i) ambient air concentration measurements, for calibration; (2) verification: (a) independent set of meteorological data (see above); (b) independent set of ambient air concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC 1100 or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency, model available on magnetic tape from NTIS in conjunction with other UNAMAP models; (2) availability of model documentation: model write-up describes: (a) theory; (b) data deck format; (c) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through geometry and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) type of output: (a) ambient concentration for any non-reactive residual; (2) values given at: (a) user-specified points; (b) specific hours (corresponding to hours for which data are input); (3) format: (a) tabular printout; (4) special features: (a) receptor contribution analysis for each of six source categories (see "model input requirements", above)
Costs	(1) model acquisition: (a) magnetic tape including PAL and other UNAMAP models is available at a cost of about $300; (2) model set-up: (a) program set-up, test case, and de-bug could normally be accomplished within a few man-days; (3) data preparation: (a) acquisition and preparation of meteorological data could normally be accomplished within a few man-days; (b) developing the layout and co-ordinates of sources and receptors could normally also be accomplished within a few days provided site base map is available; (4) actual computation: (a) typically a few dollars or so; (5) output analysis: (a) validation and verification could each respectively be performed in one man-week
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model tries to represent complicated microscale geometric relationships between point receptors and point, line, and area sources; (b) simplifying assumption: homogenous Gaussian diffusion over area, building wake effects not considered; (2) model accuracy: is expected to be comparable to "generic" Gaussian models, but model requires validation with field data because of the small scale of application and because of numerical calculational approximations employed; (3) model sensitivity: sensitivity has not been studied, but on this scale of application, model expected to be very sensitive to accuracy of wind direction data, the initial plume dimensions assumed, and the plume rise
Other Comments	(1) model limitations/restrictions: (a) model solely intended for small scale application in level terrain to study impacts upon air quality in immediate vicinity of shopping centers, parking lots, highways, airports; (b) model intended for "short term" and "worst case" analysis up to 24 hours; (c) technical details of model calculations rather difficult to understand; (2) special features: (a) model is unique in its comprehensive geometry; (b) model allows for several very specialized applications: horizontal curved line sources, "nonuniform" line sources with residualsdischarge rate varying from one end to the other, line source with varying height from one end to other; (c) submodel computes plume rise from Briggs formula, (d) model available only as part of EPA UNAMAP series; (3) application experience: (a) very limited to date

Table 5A-9. **Summary** of Single Source Model (CRSTER)

Characteristic	Summary Data
Terrain Characteristics	(1) intended for use in all types of terrain, subject to general limitations of Gaussian models in complex terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated
Time Properties	(1) time variability of inputs: (a) residuals discharges may be "steady state" annual average values, or monthly average values; (b) other stack parameters (exit velocity, temperature) may be "steady state" annual average or monthly average values; (c) meteorological data inputs are "steady state", but may vary from hour to hour; (2) time period of outputs: (a) long term: annual average; (b) short-term: (maximum) 1 hr. and 24 hr. concentrations and frequency statistics for 1 hr. and 24 hr. periods
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) 180 receptor points; (4) resolution: (a) inputs: multiple stack residuals discharges (up to 19) as a single point source, point meteorological data; (b) outputs: point ambient concentrations
Input Data Requirements	(1) initial set-up: (a) point residuals discharges for up to 19 stacks; (b) stack parameters: gas exit velocity, gas temperature, stack exit diameter, physical stack height; (c) plant elevation; (d) surface meteorological date: National Climatic Center one year magnetic tape of representative hourly airport observations for wind direction, wind speed, temperature, cloud cover, ceiling height; (e) upper air meteorological data: one year of punched cards containing 7:00 a.m. mixing height and 2 p.m. mixing height data from representative airport station (available on tape or as printed table from National Climatic Center); (f) surface meteorological station latitude and longitude and time zone; (g) receptor "ring" downwind distances; (h) receptor point elevations; note: model validation/verification procedures different from most other models, see "general comments"
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC 1100 or IBM 360; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency, model available on magnetic tape from NTIS in conjunction with other UNAMAP models, model statement listing available in user's manual; (2) availability of model documentation: user's guide available containing: (a) theory; (b) subroutines; (c) data format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) printed table of the highest ambient concentration at each of the 180 receptors for each averaging period (1 hr., 24 hr, annual and one other optional); (b) the maximum highest concentration at any receptor for each averaging period (from "a" above); (c) printed table of the second-highest concentrations at each of the 180 receptors for each averaging period except the annual; (d) the maximum second-highest concentration at any receptor for each averaging period except the annual; (e) a ranking of the 50 highest concentrations for the entire year for each averaging period except the annual; (2) special features: (a) receptor contribution may be requested optionally for the contributions of up to 10 sources to the concentrations and up to 20 receptors for averaging period for each day; (b) an optional magnetic tape for all 1 hr., 24 hr. and annual average calculations; (c) optional listings of data inputs
Costs	(1) model acquisition: (a) magnetic tape including CRSTER and other UNAMAP models costs about $300, printed listing of model (in user's guide) available for a few dollars from NTIS; (2) model set-up: (a) program set-up, de-bug and test case could normally be accomplished within a man-week or so if UNAMAP program tape is used, setting up program probably requires at least a few man-weeks if card deck is used; (3) data preparation: (a) meteorological data acquisition from National Climatic Center requires little effort (but perhaps some lead time); (b) analysis/examination of surface and upper air meteorological data may require a few man-days; (c) keypunching of upper air meteorological data would routinely require a few man-days (for use with UNAMAP program magnetic tape), keypunching the complete program will require a man-week or so; (4) actual computation costs: depends upon number of sources and options specified, but should be less than $25; (5) output analysis: special model validation procedures required, normally could be accomplished in one man-week
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model provides highest and second-highest concentrations at given receptor points for 1 hr., 24 hr. and other time periods; (b) simplifying assumptions: homogenous Gaussian diffusion, invariant mean wind direction, plume impingement upon elevated terrain; (2) model accuracy: as a result of tests of the model predicted maxima versus ambient measured concentration maxima, it is found that: (a) model accuracy varies considerably with plant location area and from receptor to receptor within area; (b) highest and second-highest concentrations are generally within a factor of 2 (though up to a factor of 5); (c) model has a tendency to underpredict, particularly at larger distances; (3) model sensitivity: (a) fairly detailed study of sensitivity indicated that the relative model sensitivity to a given variable varies from receptor to receptor, and that among the stack parameters model is most sensitive to stability class; (b) unfortunately combinations of variables were not examined, nor the sensitivity to plume rise, which is dependent on several stack paramete
Other Comments	(1) model limitations/restrictions: (a) although model prints out annual average concentrations, the invariant wind assumption would likely cause large systematic overestimations; (b) although model has been applied in complex terrain, it is better suited to gently rolling terrain; (2) special features: (a) one of the first models to provide concentrations of highest, second-highest and frequency distribution statistics: (b) model validation involves plotting the cumulative frequency of all predictions against the cumulative frequency curve of all ambient measurements at each receptor for all averaging times;[a] (c) model is well documented and described in user's guide, which describes model comparison studies against measured data and model sensitivity studies; (3) application experience: model has been applied to power plants in Massachusetts, Ohio, and Kentucky

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[a] Except for annual average applications.

Table 5A-10. Summary of Air Pollution Research Advisory Committee Model 1A (APRAC 1A)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly calculations for a user-specified period of time
Space Properties	(1) dimensionality: (a) two; (2) spatial scale of application: (a) mesoscale for areawide submodel; (b) microscale for "street canyon" submodel; (3) discretization: (a) one layer; (b) concentrations calculated at user-specified number of grid points with a user-specified grid size; (4) resolution: (a) inputs: area source and line source vehicular traffic data, point source meteorological data; (b) outputs: point carbon monoxide concentrations
Input Data Requirements	(1) initial set-up and validation: (a) vehicular traffic data for links and grids; (b) meteorological data: maximum daily temperature, minimum daily temperature, temperature and atmospheric pressure sounding for available height levels, hourly surface wind speed, wind direction, cloud cover and temperature; (c) ambient concentration measurements; (d) source coordinates; (e) receptor coordinates; (2) verification: (a) traffic data; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) for use in interactive mode a terminal is required; (b) for use in batch mode a digital computer is required; (3) computer characteristics: (a) CDC 6400 or IBM 360/50 computer; (b) typically 45,000 words of memory are required
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available with: (a) theory; (b) subroutines; (c) data deck format; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient carbon monoxide concentration; (2) values given at: (a) specific user-selected ground-level point or grid location; (b) two possible heights in "street canyon;" (3) format: (a) tabular printout; (b) punched cards; (c) magnetic tape; (d) space plots; (e) time plots; (f) frequency statistics for time period of computer run
Costs	(1) model acquisition: (a) public, nominal cost (about $7) for "as is" model and user guide (2) model set-up: (a) program set-up and keypunch: 10 man-days (estimated); (b) program de-bug: 10 man-days (estimated); (3) data preparation: (a) development of traffic information for link/grid system on suitable base map is dependent upon size of city, and state of data collection; (b) coding traffic information into link/grid system again varies but at least 10 man-days required; (c) compiling hourly meteorological data and radiosonde data requires two or three man-days (estimated); (4) actual computation time varies with size of city, number of receptors, computer output form, but typical processor time on CDC 6400 is 18 to 200 sec.; (5) output analysis: (a) graphics printing costs not specified; (b) analysis of results: overall validation or verification of composite model could be accomplished in five man-days (estimated)
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: fixed point meteorological data do not describe micrometeorological variations within city except for "street canyons," "street canyon" submodel attempts to account for localized aerodynamic effects in city core, model attempts to account for "extraurban," "intraurban," and "localized" discharges and diffusion; (b) simplifying assumptions: Gaussian diffusion (except in "street canyon"), homogeneous diffusion; (2) model accuracy: (a) overall accuracy based upon correlation coefficients is "fair"; (b) model apparently tends to underestimate concentrations below 7 or 8 ppm and overestimate at higher values; (3) model sensitivity: (a) model not very sensitive to changes in mixing height; (b) model sensitive to wind speeds and stability; (c) model may be sensitive to spatial resolution of discharges and scale of discharges included, but does not appear to have been evaluated with respect to these variables
Other Comments	(1) model limitations/restrictions: (a) model designed for carbon monoxide only; (b) model is quite comprehensive, seems to be more complex than required for localized highway problems; (2) special features: (a) "street canyon" submodel is a unique "first-cut" at modeling aerodynamic effects; (b) the "combined" model consists of subroutines to calculate residuals discharges, mixing heights, atmospheric stability, and diffusion which appear to be difficult to separate; (3) application experience: (a) model use has been fairly limited, model tests have been reported for San Jose and St. Louis; (4) new version, APRAC 2, has been recently developed: (a) also calculates HC_x and NO_x discharges and ambient concentrations (in addition to CO); (b) accept (direct) inputs of mixing heights and multiple point wind data; (c) has optional outputs of residuals discharges; (d) test results of APRAC 2 model performance have not been reported

Table 5A-11. Summary of PTMAX Model

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly or "instantaneous"
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (4) resolution: (a) inputs: single point residuals discharges source, point meteorological data (actual or hypothetical); (b) outputs: single maximum concentration and downwind point of occurrence for input meteorological and discharge conditions
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data (actual or hypothetical): wind speed, stability class; (d) several ambient concentration measurements*
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) for use in interactive model a terminal is required; (b) for use in batch mode a computer is required to run magnetic tape; (3) computer characteristics: (a) magnetic tape characteristics: 9 track, 800 bits per inch, EBCDIC code, odd parity; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting agency: (a) public agency; (2) availability of model documentation: (a) as one of the EPA UNAMAP models, PTMAX has brief write-up and test case, theory not presented in detail; (3) expertise required: (a) for batch mode, computer programmer to set-up magnetic tape; (4) model user qualities: (a) understanding of model principles, assumptions, and limitations
Output and Output Format	(1) types of output: (a) maximum downwind concentration of SO_2, suspended particulates, NO_2, HC_x, CO and downwind distance, for a given input combination of stability class and wind speed; (2) value given at single point; (3) format: tabular printout
Costs	(1) model acquisition: (a) public, "as is" model available on magnetic tape as part of the UNAMAP series; cost for the series is about $175; (2) model set-up: program set-up and test case should require a few days (estimated)
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) model not recommended for "rough" terrain unless modified; (b) simplifying assumptions: steady-state homogeneous Gaussian diffusion; (2) model accuracy: (a) normally expected to have a factor of three accuracy; (3) model sensitivity: (a) known to be sensitive to effective stack height, wind speed, and stability class
Other Comments	(1) model limitations/restrictions: (a) very specialized air quality model in that it can be used to examine hourly or instantaneous maximum concentrations and distance downwind from a single source under specified conditions of wind speed and stability (thus can be used to find a "worst combination" of meteorological conditions and resulting concentration from the source); (2) special features: (a) available as part of the UNAMAP package; (b) available in interactive mode; (c) uses the Briggs plume rise formula; (3) application experience: (a) model has been used as a preliminary screening tool

*This model, which gives estimates for a single point, would not normally be calibrated or verified in actual application, but rather would be used for planning or design purposes to find a "worst case" impact.

Table 5A-12. Summary of PTDIS Model

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic: (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly or "instantaneous"
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (4) resolution: (a) inputs: single point residuals discharges source, point meteorological data (actual or hypothetical); (b) outputs: point ambient concentrations at user-specified distances
Input Data Requirements	(1) initial set-up and validation:* (a) residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data (actual or hypothetical): wind speed, ambient temperature, stability class, mixing height; (d) several ambient concentration measurements;* (2) verification: (a) residuals discharges data; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) for use in interactive mode, a terminal is required; (b) for use in batch mode, a computer is required to run magnetic tape; (3) computer characteristics: (a) magnetic tape characteristics: 9 track, 900 bits per inch, EBCDIC code, odd parity; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting agency: (a) public agency; (2) availability of model documentation: (a) as one of the EPA UNAMAP models, PTDIS has brief write-up and test case, theory not presented in detail; (3) expertise required: (a) for batch mode, computer programmer to set up magnetic tape; (4) model user qualitites: (a) understanding of model principles, assumptions, and limitations
Output and Output Format	(1) types of output: (a) ambient centerline concentrations of SO_2, suspended particulates, NO_2, HC_x, CO at user-specified distances for given input combinations of wind speed and stability class; (2) values given at: user-specified points; (3) format: (a) tabular printout
Costs	(1) model acquisition: (a) public, "as is" model available on magnetic tape as part of UNAMAP series, cost for the series is about $175; (2) model set-up: program set-up and test case should require a few man-days (estimated)
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) model not recommended for "rough" terrain or long distances unless modified; (b) simplifying assumptions: steady-state, homogenous Gaussian diffusion, no wind speed increase with height; (2) model accuracy: (a) normally expected to have a factor of three accuracy; (3) model sensitivity: known to be sensitive to effective stack height, wind speed, and stability class
Other Comments	(1) model limitations/restrictions: (a) used to analyze downwind centerline concentrations from a single source under specified wind speed and stability conditions; (2) special features: (a) available as part of UNAMAP package; (b) available in interactive mode; (c) option to printout isopleths is convenient feature for plotting spatial concentration maps; (d) uses Briggs plume rise formulae; (3) application experience: (a) model has been used primarily as a first-cut or screening tool

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[*] This model, which is applied to a single residuals discharge source, is frequently used for planning or design purposes, without validation or verification, to examine the impact during "worst case" meteorological conditions.

Table 5A-13. Summary of PTMTP[*] Model

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (b) quasi-steady-state (user may vary source discharge or meteorological conditions for subsequent hourly periods); (2) time period of outputs: (a) short-term: hourly or instantaneous
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) number of receptors: up to 30 user-specified receptor points; (4) resolution: (a) inputs: up to 25 point residuals discharges, point meteorological data (actual or hypothetical); (b) outputs: point ambient concentrations at the user-specified receptor points
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data (actual or hypothetical): wind speed, wind direction, ambient temperature, stability class, mixing height; (d) several ambient concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) several ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) for use in interactive mode, a terminal is required; (b) for use in batch mode, a computer is required to run magnetic tape; (3) computer characteristics: 9 track, 800 bits per inch, EBCDIC code, odd parity; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: (a) as one of EPA UNAMAP models, PTMTP has brief write-up; (b) test case theory not presented in detail; (3) expertise required: (a) for batch mode: computer programmer to set-up magnetic tape; (b) research assistant; (4) model user qualities: (a) understanding of model principles, assumptions, and limitations
Output and Output Format	(1) types of output: (a) ambient concentration of SO_2, suspended particulates, NO_2, HC_x, CO; (2) values given at: (a) user-specified receptor points; (b) hourly time periods; (c) time period averages up to 24 hours;[**] (3) format: tabular printout
Costs	(1) model acquisition: (a) public, "as is" model available on magnetic tape as part of UNAMAP series, cost for the series is $175; (2) model set-up: program set-up and test case and de-bug should require several man-days (estimated); (3) data preparation: (a) data acquisition: less than a couple of man-days (estimated); (b) keypunched or recorded: a couple of man-days (estimated); (4) actual computation time: a few dollars (estimated); (5) analysis of results: validation and verification could each be performed within a few man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) model not recommended for "rough" terrain or long distances unless modified; (b) simplifying assumptions: steady-state, homogeneous Gaussian diffusion: no wind speed increase with height; (2) model accuracy: (a) normally expected to have a factor of three accuracy; (3) model sensitivity: (a) known to be sensitive to effective stack height, wind speed, and stability class
Other Comments	(1) model limitations/restrictions: (a) used to analyze ambient concentrations from point sources only; (b) used for "short-term" concentrations only; (2) special features: (a) available as part of UNAMAP package; (b) available in interactive mode; (c) uses Briggs plume rise formula; (d) interactive mode can be used in conjunction with Gifford-Hanna area source diffusion model to obtain a rapid estimate of "short-term" concentrations; (3) application experience: (a) model has been widely used, but only published test results indicated predicted concentrations were generally within a factor of three near Denver

[*] Model is also well-suited to use for preliminary analysis.

[**] Interactive mode option ensures repeated calculations for successive hours and a "time-averaged" concentration over several hours, if desired.

Table 5A-14. Summary of Gaussian Evaluation Model (GEM)

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain, except where there are severe localized distortions to dominant area wind flows
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) decay
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly ambient concentrations, averaging periods up to 24 hours
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) meso; (3) discretization: (a) one layer; (b) up to 100 user-specified receptor locations; (4) resolution: (a) inputs: residuals discharges, meteorological data as point data; (b) outputs: ambient point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) multiple point source residual discharges; (b) stack parameters: stack height, temperature, stack gas flow rate; (c) meteorological data vary somewhat with calculational options chosen (see model accuracy): some combination of hourly stability class, hourly horizontal standard deviation of wind direction, hourly horizontal wind direction change with height, hourly wind speed, mixing height; (d) decay rates of residuals; (e) surface roughness parameter; (f) ambient air quality concentrations; (g) receptor co-ordinates; (2) verification: (a) independent set of meteorological data; (b) independent set of ambient concentrations
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/168 or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: final report and user's guide available which describe: (a) theory; (b) subroutines and model options; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical abilities through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model output or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentration; (2) values given at: (a) specific points; (b) hourly averages, or time period averages not to exceed 24 hrs.; (3) format. (a) tabular printout
Costs	(1) model acquisition: (a) model user's guide, final report and listing available at no charge; (2) model set-up: (a) program set-up and debug could be accomplished within a few man-weeks; (3) data preparation: (a) data acquisition and preparation could be obtained within a few man-days; (b) keypunching of data could be accomplished within a few man-days; (4) actual computation: (a) typically $20 or so; (5) output analysis: (a) validation and verification could each be performed within a man-week or so
Model Accuracy and Sensitivity	(1) representativeness to prototype system: as a Gaussian point source model intended for application in complex terrain, GEM provides several options for calculation of key parameters, generally to allow for realism or conservatism in estimates: (a) three options for plume rise formula, or plume rise may be user-specified; (b) mixing height can be assumed to remain horizontal or to be displaced upward over elevated terrain; (c) four variations for treatment of elevated plume position in relation to elevated terrain; (d) three variations for treating effect of complex terrain upon horizontal diffusion parameter, or value may be user-specified; (e) three options for including effects of terrain surface roughness upon vertical diffusion parameter, or value may be user-specified; (f) two options for treatment of limited mixing condition; (2) model accuracy: (a) although model developers made considerable attempts to test their model over complex mountainous terrain and coastal terrain, it is clear that much more validation is needed, in part because the model has so many combinations of options; (b) model developers concluded that the model seemed to work somewhat better in the inland mountainous rather than the coastal terrain, that vastly different results were obtained depending upon the combination of model options chosen, and that it appears that (with good judgment in selection of options) the Gaussian formulation can predict the hourly maximum concentration within a factor of two and the downwind distance within a factor of two during unstable atmospheric conditions; (3) model sensitivity: although this topic was not formally studied, it is clear that: (a) ambient concentrations are quite sensitive to the different options for treating plume position in comparison to elevated terrain and to the treatments selected for calculating horizontal and vertical diffusion parameters; (b) model is insensitive to option selected for limited mixing
Other Comments	(1) model limitations/restrictions: (a) model not suitable where there are large variations in wind direction (such as within complex canyon and in coastal regions); (b) model not intended for "long-term" annual average applications; (2) special features: (a) ability to accept user-specified data is important feature; GEM model could incorporate empirically derived plume parameters from tracer or plume photography studies; (b) model developers have attempted to include best available options to account for terrain elevation and roughness effects; (3) application has been applied to a smelter in Utah and power plant in California, both in complex terrain

Table 5A-15. Summary of Argonne Puff Model

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) chemical decay
Mathematical Processes	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerical integration subroutine used to facilitate solution of integrated puff equation
Time Properties	(1) time variability of inputs: (a) dynamic, parameters allowed to vary from hour to hour ("piecewise constant"); (2) time period of outputs: (a) short term: daily or shorter periods
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) user-specified number of grids and grid size or standard program grid size option; (c) number of receptors defined by the vertices of the area source grid; (4) resolution: (a) inputs: residuals discharge data as point sources or "virtual" area (volume) sources, meteorological point data; (b) outputs: ambient concentration (grid) points
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges, point, and area; (b) stack parameters: height, heat emission rate = f(diameter, exit velocity, temperature); (c) meteorological data: hourly wind speed and direction, stability, mixing height; (d) several ambient concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharge data; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: digital computer; (3) computer characteristics: (a) IBM 360-75 or equivalent; (b) program language: FORTRAN
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: program description and listing available containing: (a) basic theory; (b) subroutines; (c) partial test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through advanced calculus; (b) knowledge of specialized model solution techniques; (c) specialized knowledge of model principles, assumptions, and limitations; (d) prior experience with puff trajectory models desirable, otherwise access to consultations mandatory
Output and Output Format	(1) types of output: (a) ambient concentration of SO_2 and suspended particulates for various time periods; (2) values given at: (a) grid locations; (3) format: (a) tabular printout; (b) time series plots
Costs	(1) model acquisition: (a) public, "as is" listing free; (2) model set-up: (a) program set-up: two man-weeks (estimated); (b) test case: one man-week (estimated); (c) de-bug: one man-week (estimated); (3) data preparation: (a) data acquisition: one man-week (estimated); (b) analysis and reduction: up to one man-week (estimated); (c) recording and keypunching: up to a few man-days; (4) actual computation: expensive relative to other Gaussian (non-puff) grid models; (5) output analysis: (a) printout/plotting expenses difficult to specify; (b) analysis of results: validation and verification effort varies, at least one man-week for each is estimated
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: if multiple point wind speed and direction data are available within city, more accurate plume trajectories can be simulated, nevertheless the approximate accuracy of trajectories and spatial variations in residuals discharges can cause considerable errors in predicted concentration at given points and times; (b) simplifying assumptions: Gaussian puff has equal x and y dimensions, upwind source contributions greater than six grid areas are neglected, initial grid area sources represented by three-dimensional virtual source; (2) model accuracy: (a) model seems to be better at predicting the likelihood of "episode" concentrations rather than the actual concentrations; (b) ironically, model predicted Chicago mean seasonal values quite well for given locations, but has considerable scatter in short-term concentration predictions (extensive published validation results available for Chicago); (3) model sensitivity: individual hourly trajectories sensitive to errors in wind direction, model concentrations also sensitive to plume rise calculations
Other Comments	(1) model limitations/restrictions: (a) presence of complicated flow patterns, such as lake breeze, may preclude use of model; (2) special features: (a) trajectory puff model intended for application during low wind speed conditions which pose theoretical problems for Gaussian plume models; (b) model has been used in a number of land use planning and "episode" control studies by the model developers; (c) although model is intended for "short-term" concentrations, it seems to give excellent long-term predictions from repeated applications, while short-term predictions are comparable to simpler models; (d) pure natural systems model; (3) application experience: (a) model has been used extensively in Chicago area

Table 5A-16. Summary of VALLEY Model

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain, particularly intended for valley and mountain areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) decay
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: seasonal or annual average; (b) short-term: twnety-four hour average concentrations
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) 112 receptor points, partially specified by user; (4) resolution: (a) point and area residuals discharges, single point meteorological data; (b) point ambient concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point and area residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity, and volume flow rate; (c) meteorological data: joint frequency of wind speed (six categories), wind direction (sixteen classes), and stability class (six classes), annual average or seasonal mixing heights; (d) several ambient concentration measurements; (e) source coordinates; (f) receptor coordinates; (g) receptor heights; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC 1110 or equivalent; (b) 56,000 words of memory; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available with (a) theory; (b) subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (3) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) considerable modeling experience required for successful application of VALLEY model for short-term concentration in complex terrain
Output and Output Format	(1) types of output: (a) ambient concentrations of SO_2, suspended particulates, toxic metals, and other nonreactive residuals; (2) values given at: (a) receptor points; (b) daily seasonal or annual time periods; (3) format: (a) concentration maps from individual sources and summed total concentration map for all sources
Costs	(1) model acquisition: (a) model listing and user guide available "as is" from NTIS for nominal cost and available on magnetic tape as part of EPA UNAMAP series; (2) model set-up: (a) to set-up card deck program, 10-15 man-days (estimated); (b) test case and de-bug (10-15 days) estimated; (3) data preparation: (a) if National Climatic Center "Star" Data are used, data analysis and reduction would require only a few man-days; (b) keypunching and recording would only require 2-3 man-days; (4) actual computation: (a) single source short-term problem would not cost more than a few dollars; (b) multiple source long-term problem might cost $10-15; (5) analysis of results: (a) validation and verification could each be performed in about one man-week
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: allows for variation in receptor heights, allowsfor multiple plume reflections from surface, uses fixed point meteorological data, includes virtual area source approximations; (b) simplifying assumptions: during stable conditions plume is assumed to approach elevated terrain receptor to within 10 meters of surface, during unstable or netural conditions plume assumed to maintain initial height relative to ground, "sector-averaged" plume spread assumed for both "long-term" and "short-term" applications in complex terrain; (2) model accuracy: (a) model tests have been reported only for 24 hour estimated concentrations; from limited test the majority of estimates was within a factor of two of the observed "second highest" 24 hour concentration, at two sites estimates were much higher than observed; (3) model sensitivity: not reported, but short-term estimates are obviously highly sensitive to "worst case" meteorological data as determined by user's judgment
Other Comments	(1) model limitations/restrictions: (a) model application requires careful meteorological data selection for "short-term" worst case and experienced judgment; (b) analysis of multiple sources is rather cumbersome and difficult to interpret; (c) selection of steady-state conditions during a six-hour period to represent worst 24 hour period is rather arbitrary; (2) special features: (a) model contains a plume rise subroutine; (b) model routinely provides concentration map outputs; (3) application experience: (a) model has been applied to estimate "worst case" 24 hour SO_2 concentrations in the vicinity of four smelters in Arizona and Utah

Table 5A-17. Summary of Oak Ridge Fog and Drift Model (ORFAD)

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) condensation of water vapor (2) evaporation of drift droplets
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, modified Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: annual average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) up to nineteen user-specified distances for sixteen compass directions; (4) resolution: (a) inputs: point residuals discharge data; point meteorological data; (b) outputs: point environmental quality indicators (see outputs below)
Input Data Requirements	(1) initial set-up:[a] (a) residuals discharges: mass fraction of circulatory water discharged as drift, concentration of dissolved solids in circulating water, class sizes of drift particles; (b) stack parameters: circulating water temperature change, circulating mass flow rate, inside cooling tower radius at top of tower, exit velocity of tower discharges at top of tower, heat discharge rate, height of tower; (c) meteorological data: National Climatic Center weather tape containing multiple years of wind speed and direction, dry and wet bulb temperatures, total cloud cover, cloud ceiling and natural fog; (d) source coordinates
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 360/91 or equivalent; (b) program language: FORTRAN IV (Level H)
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's manual available with (a) theory; (b) subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through basic calculus is desirable; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient air concentration of solids; (b) total additional hours of fog produced; (c) total hours of ice produced; (d) number of hours of fog at discrete receptors; (e) number of hours of ice at discrete receptors; (f) annual deposition rate of drift dissolved solids; (2) values given at: (a) user selected receptor points; (b) annual time periods; (3) format: (a) tabular printout; (b) optional fog or drift deposition CALCOMP map; (c) optional vertical plane map of fog occurrences
Costs	(1) model acquisition: (a) public, "as is" model documentation and listing available for $6 from National Technical Information Center; (2) model set-up: (a) program set-up and keypunch: 15 man-days (estimated); (b) test case and de-bug: 10 man-days (estimated); (3) data preparation: (a) analysis and reduction: 3 man-days (estimated); (c) keypunched or recorded: 1-3 man-days, depending upon number of analyses and years of meteorological tape data; (4) actual computation: (a) for one cooling tower or group of cooling towers and several years of meteorological data costs are roughly $100-200; (5) output analysis: (a) if complete tabular printout desired for every year, cost increases substantially; (b) analysis of results is normally accomplished within a couple of days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) Hanna modification of Briggs plume rise equation accounts for plume buoyancy due to vapor density and latent heat, drift deposition includes evaporative effects; (b) simplifying assumptions: evaporation occurs in discrete stages as function of relative humidity, fog begins at 100% relative humidity, "steady-state" discharge conditions over meteorological period; (2) model accuracy: not reported; (3) model sensitivity: not reported, but outputs are probably quite sensitive to plume rise calculations and to evaporation calculations
Other Comments	(1) model limitations/restrictions: (a) model limited to cooling towers only; (b) model limited to a single cooling tower or group of towers which can be treated as a single point source; (c) model intended for annual averages; (2) special features: (a) model has subroutine to calculate plume rise from Hanna-Briggs formula; (b) model has subroutine to calculate evaporation effects from Hosler, Pena, and Pena results; (3) model experience: (a) has been used primarily for rough environmental impact analyses of power plant cooling towers for rather rough analyses (normally without validation and verification)

[a] Model is generally used as a preliminary or "screening tool" without validation or verification.

Table 5A-18. Summary of Atmospheric Transport Model

Characteristic	Summary Data
Terrain Characteristics	(1) smooth or gently rolling; (2) valley or basin; (3) mountainous; (4) forest
Physical Processes	(1) transport; (2) diffusion; (3) dry deposition: (a) impaction; (b) gravitational settling; (4) wet deposition (washout)
Chemical Processes	(1) no chemical processes explicitly included
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: seasonal, annual average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) mero; (3) discretization: (a) one layer; (b) up to ten grid area sources of user-specified size; (c) up to ten user-specified receptors; (4) resolution: (a) inputs: residuals discharges as point, line, or area sources, point meteorological data; (b) outputs: point ambient concentrations and deposition rates
Input Data Requirements	(1) initial set-up and validation: (a) point, line, and area residuals discharges; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data: joint frequency of wind speed (up to eight classes), wind direction (sixteen directions), and stability class (six classes); (d) rainfall rates; (e) ambient concentration measurements; (f) ambient deposition measurements; (g) source coordinates; (h) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements; (d) ambient deposition measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) model intended for most IBM, CDC, and UNIVAC computers; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational models and supporting information: (a) public agency; (2) availability of model documentation: user guide available with (a) theory; (b) subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of output: (a) ambient concentrations of SO_2, suspended particulates, nutrients, and toxic metals; (b) deposition rates of same residuals; (2) values given at: (a) user-specified points; (b) user-specified months, seasons, or annual time periods
Costs	(1) model acquisition: (a) public, "as is" model listing and user document available free of charge; (2) model set-up: (a) program set-up and keypunch: 10 man-days (estimated); (b) test case and de-bug: 10 man-days (estimated); (3) data preparation: (a) analysis and reduction: 3 man-days (estimated); (b) keypunched and recorded: 2 man-days (estimated); (4) actual computation: cost not available, but should be only a few dollars because of limited numbers of receptors and sources; (5) output analysis: calibration and verification could each be routinely performed in five to ten days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: fixed single point meteorological data; deposition calculations include a terminal velocity for particulates or an arbitrary "default" deposition velocity, whichever is larger, for gases an arbitrary deposition velocity is used; diffusion parameter curves have been extended to 50 kilometer distance with use of Briggs and Smith curves; (b) simplifying assumptions: Gaussian diffusion, homogeneous diffusion, homogeneous deposition velocity; (2) model accuracy. (a) fairly good statistical correlations and accuracy, generally within a factor of 2, have been reported for ambient concentration, accuracy of deposition rates has not been reported; (3) model sensitivity: not reported but deposition rates are obviously sensitive to dry deposition velocity and wet deposition washout coefficient
Other Comments	(1) model limitations and restrictions: (a) model intended primarily for limited numbers of large point sources and area sources; (2) special features: (a) has an option for theoretical or empirical values of deposition velocity, or the default value; (b) has a subroutine to compute theoretical re-suspension of particles deposited; (c) model well documented; (3) model experience: (a) has been and is being fairly widely used for deposition analyses (Wisconsin, New Mexico, Missouri, Tennessee), but test results of model have not been published

Table 5 A-19. Summary of the Research Corporation of New England Cooling Tower Model (TRC)

Characteristic	Summary Data
Terrain Characteristics	(1) model best suited to smooth or gently rolling terrain, though it has been applied in a variety of terrain types
Physical Processes	(1) transport and diffusion of water vapor
Chemical Processes	(1) water vapor condensation
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated
Time Properties	(1) time variability of inputs: (a) quasi-steady-state; (2) time period of outputs: (a) short-term: applied to individual hourly time periods to calculate formation of fog; (b) long-term: individual hours of fog summed over longer period, such as a year, to yield the total number of hours of fog at given receptor point
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) user-specified number of point receptors (and point sources); (4) resolution: (a) inputs: point source cooling system water vapor discharges, point meteorological data; (b) outputs: fog frequency at user-selected points
Input Data Requirements	(1) initial set-up and validation: (a) water vapor discharge rate; (b) cooling system parameters: height, diameter, exit velocity, exit temperature; (c) meteorological data: hourly wind speed and direction, stability, relative humidity, mixing height, fog or visibility records; (d) source coordinates; (e) receptor coordinates; (2) verification:* (a) residuals discharges; (b) meteorological data (see above)
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) proprietary: consulting services for model application may be purchased, or purchase of model and user instructions may be negotiated; (2) availability of model documentation: no formal user's guide available; (3) expertise required: (a) specialized knowledge about cooling system types and operational characteristics; (b) specialized understanding of model principles and assumptions and limitations; (c) prior experience with cooling system or access to consultations
Output and Output Format	(1) types of output: (a) frequency of fog occurrence; (2) values given at: (a) user-selected points; (3) format: (a) tabular printouts
Costs	(1) model aquisition and set-up costs cannot be specified; (2) contracting developer for typical problems normally costs several thousand dollars
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: readily available relative humidity and fog records (airport) may or may not be representative of study area, practicality dictates that a dynamic process be modeled by a quasi-steady-state process in which cooling system characteristics do not vary for long periods of time; (b) simplifying assumptions: homogeneous Gaussian diffusion; (2) model accuracy: models of this type are rarely calibrated or verified, accuracy must be regarded as very rough approximation; (3) model sensitivity: model sensitive to effective stack height, wind speed, relative humidity, stability class
Other Comments	(1) model limitations/restrictions: (a) model normally applied for a few different "scenarios" of cooling system design and related cooling system parameters, which are in turn dependent upon some representative ambient meteorological conditions, model applicable "in the long run" rather than on a given day; (2) special features: (a) model can incorporate site-specific historical fog probabilities and thus realistically note the presence of fog based on empirical relationships (at relative humidities at less than saturation); (b) combined natural systems model with plume rise submodel; (3) application experience: (a) model has been used as a screening tool without verification for analysis at numerous nuclear power plant sites

*Model used as planning or preliminary tool and not usually verified.

Table 5A-20. Summary of Texas Episodic Model (TEM)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) chemical decay may be accounted for through user-specified "half-life" of residual
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) analytically integrated, Gaussian
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) short-term: hourly to 24 hour average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) user-specified number of grids, up to 50 x 50, and grid size; (c) up to 2,500 receptor points, corresponding to grid points; (4) resolution: (a) inputs: residuals discharge data as point sources and user-specified grid area sources, point meteorological data (actual or hypothetical)
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges: point and area residuals discharge sources; (b) stack parameters: height, diameter, temperature, exit velocity; (c) meteorological data: wind speed and direction, stability class, mixing height; (d) several ambient concentration measurements; (e) residuals half-life, actual or arbitrary; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC 1100 computer; (b) program language: FORTRAN IV; (c) very fast running time due to calculational innovations
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public; (2) availability of model documentation: user's guide contains: (a) theory; (b) subroutines listing; (c) data deck format; (c) documentation test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs or access to consultations
Output and Output Format	(1) types of outputs: (a) ambient concentration of SO_2, suspended particulates, NO_2, HC_x, or CO (any two); (b) values given at: grid points; (3) format: (a) tabular printout; (b) printout "map" of receptor grids and concentrations; (c) punched cards for input to concentration plotting routines; (4) special features: (a) receptor contribution analysis (of the five largest sources impacting up to 625 receptors)
Costs	(1) model acquisition: (a) public, "as is" cost of model listing and user's guide is $20; (2) model set-up: (a) program set-up: one to two man-weeks (estimated); (b) test case: few man-days (estimated); (c) de-bug: one man-week (estimated); (3) data preparation: (a) data acquisition: a few man-days (estimated); (b) analysis and reduction: a few man-days (estimated); (c) keypunched or recorded: a few man-days (estimated); (4) actual computation time: (a) a major advantage of TEM is the fast program running time, only a few dollars per computer run are typical costs for multiple source analysis; (5) output analysis: (a) printout expense increases if plotting routines are used; (b) analysis of results: validation or verification could normally each be performed in about one man-week
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: single point meteorological data are simplification of urban and mesoscale meteorology, wind speed estimation at stack height is more representative than ground-level wind; (b) simplifying assumptions: homogeneous Gaussian diffusion; (2) model accuracy: (a) calculational short-cuts introduce an error of a few percent compared to more exact calculational methods; (b) accuracy of model expected to be similar to that for other Gaussian models; (3) model sensitivity: (a) known to be sensitive to effective stack height, wind speed, and stability class
Other Comments	(1) model limitations/restrictions: (a) model restricted to "short-term" concentrations such as "episodes;" (2) special features: (a) model combines the Gifford-Hanna model for area sources and the Gaussian plume model for point sources; (b) the use of an interpolation between "pre-calculated" parameters (rather than calculating each diffusion parameter) results in a very fast computation with minimum effect upon accuracy; (3) application experience: (a) model has been primarily applied to Texas; model test results are not published

Table 5A-21. Summary of Texas Climatological Model (TCM)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) decay "half-life"
Time Properties	(1) time variability of inputs: (a) steady-state; (2) time period of outputs: (a) long-term: seasonal, annual average
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) user-specified number and size of grid; (c) up to 100 receptors; (4) resolution: (a) inputs: point and area residuals discharges, point meteorological data; (b) outputs: point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges: point, area; (b) stack parameters: stack height, stack diameter, exit velocity, exit temperature; (c) meteorological data: joint frequency of wind speed (six classes), wind direction (sixteen directions) and stability class (six classes), annual average or seasonal mixing height; (d) several ambient concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC 1108 or equivalent
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of documentation: user guide available with (a) theory; (b) subroutines; (c) data deck format; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles, assumptions, and limitations; (c) experience in interpretation of model outputs or access to consultations
Ouput and Output Format	(1) types of output: (a) ambient concentration of SO_2, suspended particulates, NO_x, HC_x, CO (any three); (2) values given at: (a) user-specified points; (b) ground-level; (3) format: (a) tabular printout; (b) CALCOMP map; (4) special features: (a) calibration subroutine; (b) receptor contribution analysis
Costs	(1) model acquisition: (a) public, "as is" model listing and user guide available for $15; (2) model set-up: (a) program set-up and keypunch: 8 man-days (estimated); (b) test case and de-bug: 2 man-weeks (estimated); (3) data preparation: (a) analysis and reduction: 3 man-days (estimated); (b) keypunched or recorded: 2 man-days estimated; (4) actual computation: depends upon problem and number of sources, comparison indicates computation time is one to two orders of magnitude faster than CDM; (5) output analysis: (a) routine validation/verification could each be performed in one week
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: fixed point meteorological data do not describe micrometeorological variations within city nor "urban heat island" air circulations; (b) simplifying assumptions: Gaussian diffusion, homogenous diffusion, Gifford-Hanna area source diffusion calculation; (2) model accuracy: based upon somewhat limited testing for sulfur dioxide, model gave almost identical results in Houston as the CDM, accuracy for other residuals not well established; (3) model sensitivity: not published, but point source calculations are sensitive to stability class and effective stack height, while area source calculations are sensitive to wind speed
Other Comments	(1) model limitations and restrictions: (a) designed for annual average and seasonal applications; (2) special features: (a) very fast computation time, noted above, cue to short-cuts and precalculations used by program; (3) application experience: (a) limited published experience of model use--SO_2 (Houston) and suspended particulates (Dallas-Fort Worth), no published experience with respect to other residuals

Table 5A-22. Summary of International Business Machines Air Quality 1 and 2 (IBMAQ 1 and 2)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) chemical decay for sulfur dioxide
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerically integrated, finite difference
Time Properties	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) short-term: hourly to daily
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) meso; (3) discretization: (a) fourteen layers; (b) 30 x 40 grid, grid spacing is user-specified and may be variable; (4) resolution: (a) inputs: residuals discharges as area sources, multiple point wind speed and direction data, point mixing height data, multiple point ambient concentrations; (b) outputs: area grid concentrations
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges for point and area sources; (b) meteorological data: hourly multiple point wind speed and wind direction data, point mixing height; (c) ambient concentration measurements; (d) source and receptor grid area coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/195 or equivalent; (b) core storage: 96,000 words (four bytes each); (c) program language: FORTRAN IV (level H)
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: final report and user's guide contain: (a) theory; (b) subroutines; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with: (a) knowlege of code, diffusion model, and advanced mathematical solution technique; (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations of SO_2 and suspended particulates; (2) values given at: (a) grid areas; (b) up to 25 user-specified receptor points; (3) format: (a) tabular printout; (b) spatial concentration maps
Costs	(1) detailed costs are not available, except that typical computer runs for the St. Louis area cost around $40; (2) it is obvious that several months of time would be required to set-up, de-bug, and calibrate the model; the costs could be in the tens of thousands of dollars, not including the development of the residuals discharge data nor required multiple point meteorological data; (3) subsequent model applications would cost considerably less
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model subroutines compute a single "weighted" interpolated wind field from meteorological data as input to transport/diffusion model, vertical diffusivity coefficient is a function of wind speed, roughness, stability class, and height, and can vary spatially, vertical layer contains exceedingly high resolution; (b) simplifying assumptions: a single horizontal diffusion coefficient is arbitrarily assumed to be representative of region, a single mixing height is used for a region; (2) model accuracy: (a) model has corrections to reduce finite difference inaccuracies (numerical diffusion); (b) for 24 hour periods, model predictions were generally within a factor of two or three of measured sulfur dioxide concentrations, though with considerable scatter; (c) for 2 hour periods based upon data available, it is difficult to determine accuracy of model, comparisons seem to vary considerably with different monitoring stations; (3) model sensitivity: model is anticipated to be sensitive to grid size and boundary conditions
Other Comments	(1) model limitations/restrictions: (a) model has been tested in St. Louis area only and has not been tested in diverse topography; (b) model has been tested for sulfur dioxide only; (2) special features: (a) model suggests comparatively simple treatment of boundary and initial conditions; (b) model uses comparatively simple procedure to develop wind field and mixing heights; (c) the time, expense, and effort required to use model would normally suggest it be also used with other "nonreactive" residuals, e.g., particulates, possibly nitrogen oxides; (d) vertical discretization easily accommodates discharges from elevated sources, although plume rise not calculated; (e) grid model permits variable sized grid for better resolution where needed; (3) application experience: model use has been limited to St. Louis and, to a lesser extent, Venice, Italy

Note: While the basic theory and objectives remain the same in IBMAQ 1 and IBMAQ 2, the latter version was written to permit improved physical assumptions and to permit easier application. IBMAQ 2 has not yet been tested against ambient air quality data so that such discussions here are related to IBMAQ 1.

Table 5 A-23. Summary of Atmospheric Carbon Monoxide Simulation Program (ACSOP)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) "decay"
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) mathematical: numerically integrated, finite element
Time Properties	(1) time variability of inputs: (a) dynamic; (b) quasi-steady-state; (2) time period of outputs: (a) short-term: hourly
Space Properties	(1) dimensionality: (a) two; (2) spatial scale of application: (a) meso; (3) discretization: (a) one layer; (b) up to 300 grid elements of user-specified, varying sizes (shapes are triangles and quadrilaterals); (c) up to 1,000 grid receptor points: (4) resolution: (a) inputs: CO discharge as area sources, point meteorological data; (b) outputs: point ambient CO concentrations
Input Data Requirements	(1) initial set-up and validation: (a) activity information and CO discharges for mobile and stationary sources; (b) meteorological data: wind speed and direction, mixing heights; (c) diffusivity parameters, k_x and k_y ; (d) several ambient air concentration measurements; (e) source coordinates; (f) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) diffusivity parameters; (d) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) UNIVAC, IBM or Honeywell systems have been used; (b) core storage: 60,000 words; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide available with: (a) theory; (b) description of subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with: (a) knowlege of diffusion model, advanced mathematics, and finite element numerical solution technique (and its particular problem definition requirements); (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations of CO; (2) values given at: (a) user-specified grid points; (b) user-specified times; (3) format: (a) tabular printout
Costs	(1) cost estimates are not available: (a) computer costs are probably comparable to other nonreactive conservation of mass models; (2) exclusive of gathering activity and discharge information in a grid network, it would probably require a few man-months to perform the following: program set-up/keypunch, test case/program de-bug, meteorological data preparation/keypunch, grid network recording/keypunch, validation, verification
Model Accuracy and Sensitivity	(1) evaluation of model accuracy and sensitivity has not yet been published
Other Comments	(1) model limitations/restrictions: (a) model is designed for CO only; (b) model requires considerable testing before applications are undertaken; (2) special features: (a) model allows for high spatial resolution where needed and less spatial resolution where not needed; (b) similarly, model is well suited for testing the effect upon ambient concentration of different spatial resolution patterns; (c) model has optional subroutine which computes a "mass consistent" wind field from wind speed and direction inputs, or user may directly insert wind field; (d) model has optional subroutine to help find an optimal grid numbering scheme; (3) application experience: (a) model has had very limited use (Anchorage, Alaska) and model test results have not been published

Table 5A-24. Summary of Livermore Regional Air Quality Model I (LIRAQ I)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas; (2) all types of terrain
Physical Processes	(1) transport and diffusion; (2) dry deposition (through "deposition velocity")
Chemical Processes	(1) none; however, "decay" could be accounted for by changing deposition velocity if model were used with "unstable" residuals
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerically integrated, finite difference
Time Properties	(1) time variability of inputs: (a) dynamic; (b) quasi-steady-state; (2) time period of outputs: (a) short-term: from a few hours to a few days, the latter if a full "episode" analysis, including nighttime, is desired
Space Properties	(1) dimensionality: (a) two; (2) spatial scale of application: (a) meso, urban areas and regions up to about 220 km. x 250 km., depending upon resolution used; (3) discretization: (a) one layer; (b) up to a 45 x 50 grid, user has option of 1 km., 2 km., or 5 km. grid size; (c) number of receptors is equal to the number of grid elements; (4) resolution: (a) inputs: point and line source residuals discharge data and point meteorological data are "smoothed" for use with grid elements; (b) outputs: ambient air quality concentrations as grid area averages
Input Data Requirements	(1) initial set-up and validation: (a) stationary and mobile source inventory of point and nonpoint residuals discharges; (b) meteorological data: hourly multiple point wind speed and wind direction measurements, multiple point inversion height measurements; (c) two sets of multiple point ambient concentration measurements, for initial and boundary conditions and for validation, respectively; (d) source and receptor grid area coordinates; (2) verification: (a) residuals discharge data; (b) meteorological data, as noted above; (c) two sets of ambient concentration measurements, as noted above
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) CDC 7600 or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide, project reports, and appendices contain: (a) theory; (b) subroutines (on microfiche); (c) program files; (d) test case (the interactive mode example used for San Francisco Bay Area); (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with (a) knowledge of code, diffusion model, and advanced mathematical solution techniques; and (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ground-level ambient concentration of CO; (b) vertically-averaged ambient concentration (through mixing layer); (c) inversion height spatial fields; (d) wind speed and direction spatial fields; (2) values given at: (a) grid elements; (b) hourly intervals; (3) format: (a) tabular printouts for ground-level and vertical concentrations and meteorological fields; (b) maps for ground-level and vertical concentrations and meteorological wind fields and inversion heights; (c) time plots for receptor/grid element ground-level and vertical concentrations
Costs	(1) detailed costs are not available, except that typical computer runs for 24 hour periods for the San Francisco Area would require about ten minutes to one hour of computation time at a cost of $100-$500; (2) it is obvious that many months of time would be required to set-up, de-bug, and validate the model, not including the extensive residuals discharge inventory nor the extensive multiple point meteorological data collection required; (3) subsequent model applications would cost considerably less
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model includes topographical variations, model subroutine produces consistent wind field and inversion heights as input to transport/diffusion model, model incorporates a deposition sink term (deposition velocity); (b) simplifying assumptions: a single "vertically-averaged" concentration is representative of concentrations above ground-level, horizontal diffusion coefficient variation with height is negligible, horizontal and vertical diffusivity coefficients vary in space, primarily as a function of wind speed; (2) model accuracy: (a) model has corrections to reduce finite difference inaccuracies ("numerical" diffusion); (b) based upon very limited testing of model predictions against measured concentrations, model accuracy for CO is dependent upon resolution used; model resolution of 5 km. produced severe underpredictions, while a 1 km. grid seemed to produce accurate area maximum and mean concentration predictions; (3) model sensitivity: (a) model concentrations found to be quite sensitive to grid resolution, boundary conditions, and inversion base heights

Table 5A-24. LIRAQ I (continued)

Characteristic	Summary Data
Other Comments	(1) model limitations/restrictions: (a) model extremely complex; (b) model originally intended for CO and has not been tested for other "nonreactive" residuals; (c) model requires large amounts of input wind speed and direction and inversion height data to utilize properly; (d) grid model does not permit very localized assessment of large point sources nor an impact assessment of large elevated point sources; (e) some reprogramming required for applications outside San Francisco Bay Area; (2) special features: (a) MASCON submodel produces mass consistent area wind speeds and directions and inversion heights from input data (thus LIRAQ I is a combined flow model and transport and diffusion model); (b) the time, expense, and effort required to set up LIRAQ I would normally suggest that it be also used for other "nonreactive" residuals, e.g., SO_2, particulates, as well as CO, and that it be used in conjunction with its companion model LIRAQ II; (c) the different resolution grids available and number of grids add versatility for analyzing how transport/diffusion processes affect practical air quality management problems on urban and interurban scales up to 200 km.; (d) informative final report (and appendices) provides many insights into modeling practices and problems and examples of how LIRAQ I can be used in practical management problems; (3) model experience: (a) model use to date has been limited to San Franciso; (b) new version of model and documentation will be available shortly with capacity for SO_2

Table 5A-25. Summary of Livermore Regional Air Quality Model II (LIRAQ II)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas; (2) all types of terrain
Physical Processes	(1) transport and diffusion; (2) dry deposition (through "deposition velocity")
Chemical Processes	(1) photochemical oxidation reactions which form ozone from precursors
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerically integrated, finite difference
Time Properties	(1) time variability of inputs: (a) dynamic; (b) quasi-steady-state; (2) time period of outputs: (a) short-term: form a few hours to a few days, the latter if a full "episode" analysis including nighttime is desired
Space Properties	(1) dimensionality: (a) two; (2) spatial scale of application: (a) meso, urban areas, and regions up to about 100 km x 100 km; (3) discretization: (a) one layer; (b) up to a 20 x 20 grid, user has option of 1 km, 2 km, or 5 km grid size; (4) resolution: (a) inputs: point and line source residuals discharges data and point meteorological data are smoothed for use with grid elements; (b) outputs: ambient air quality concentrations as grid area averages
Input Data Requirements	(1) initial set-up and validation: (a) stationary and mobile source inventory of point and nonpoint residuals discharges, including hydrocarbons and nitrogen oxides; (b) meteorological data: hourly multiple point wind speed and wind direction measurements, multiple point inversion height measurements, multiple point solar intensity measurements; (c) two sets of multiple point ambient concentration measurements: for initial and boundary conditions and for validation, respectively; (d) source and receptor grid area coordinates; (2) verification: (a) residuals discharges data; (b) meteorological data, as noted above; (c) two sets of ambient concentration measurements, as noted above
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) CDC 7600 or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide, project reports and appendices contain: (a) theory; (b) subroutines (on microfiche); (c) program files; (d) test case (the interactive mode example used for San Francisco Bay Area); (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with (a) knowledge of code, diffusion model, photochemistry, and advanced mathematical solution techniques; and (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ground-level ambient concentrations of hydrocarbons, nitrogen oxides, ozone, and carbon monoxide; (b) vertically-averaged ambient concentrations (through mixing layer): hydrocarbons, nitrogen oxides, and ozone; (c) inversion height spatial fields; (d) wind speed and direction spatial fields; (2) values given at: (a) grid elements; (b) hourly intervals; (3) format: (a) tabular printouts for ground-level and vertical concentrations and meteorological fields; (b) maps for ground-level and vertical concentrations and meteorological wind fields and inversion heights; (c) time plots for receptor/grid element ground-level and vertical concentrations
Costs	(1) detailed costs are not available, except that typical computer runs for 24-hour periods for the San Francisco Bay Area would require about three-quarters of an hour of computation time at a cost of around $350; (2) it is obvious that many months of time would be required to set up, de-bug, and calibrate the model; costs would run well in the tens of thousands of dollars, not including the extensive residuals discharge inventory nor the extensive multiple point meteorological data collection required; (3) subsequent model applications would cost considerably less
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model includes topographical variations, model subroutine produces consistent wind field and inversion heights as input to transport/diffusion model, model contains an extensive treatment of photochemistry, model incorporates a deposition sink term (deposition "velocity"); (b) simplifying assumptions: a single "vertically averaged" concentration is representative of concentrations above ground-level, horizontal diffusion coefficient variation with height is negligible, horizontal and vertical diffusivity coefficients vary in space, primarily as a function of wind speed; (2) model accuracy: (a) ability to correct for finite difference inaccuracies is more limited in LIRAQ II than in LIRAQ I; (b) nevertheless, based upon very limited testing of ozone predictions in a 5 km grid versus measured concentrations, comparisons were generally very close (and all comparisons were within a factor of two); (c) again using a 5 km grid, predictions for nitrogen oxides and hydrocarbons were somewhat inconclusive in the sense that one day showed underpredictions, while another showed overpredictions; (3) model sensitivity: (a) model ozone predictions were found to be quite sensitive to the solar radiation intensities, though not sensitive to temperature and humidity; (b) all photochemical products were found to be sensitive to boundary conditions used; (c) sensitivity of photochemical product concentrations to different grid sizes was not investigated

Table 5A-25. LIRAQ II (continued)

Characteristic	Summary Data
Other Comments	(1) model limitations/restriction: (a) model extremely complex; (b) grid model requires large amounts of input wind speed and direction and inversion height data to utilize properly; (c) the core storage requirements for solving the photochemistry limit the grid size to 20 x 20, which in turn limits the area size and/or resolution; (d) the model does not permit very localized impact assessment of large point sources nor an impact assessment of large elevated point sources; (2) special features: (a) MASCON submodel produces mass consistent wind speeds and directions and inversion heights from input data (thus LIRAQ II is a combined flow model and transport and diffusion model); (b) informative final report (and appendices) provides many insights into modeling practices and problems and examples of how LIRAQ II can be used in practical management problems; (3) applications experience: (a) model use to date has been limited to San Francisco Bay Area, application of model to St. Louis is commencing; (4) new version of model and documentation will be available shortly with added features: (a) capability for SO_2 and sulfates; (b) updated photochemical mechanism

Table 5A-26. Summary of Reactive Plume Model (RPM)

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) photochemical oxidation processes for formation of ozone, nitrogen oxides, and sulfates
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerical integration
Time Properties	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) daily or hourly
Space Properties	(1) dimensionality: (a) one; (2) spatial scale of application: (a) meso (up to 100 km.); (3) discretization: (a) one layer; (b) parcel trajectory for single point sources; (4) resolution: (a) inputs: point residuals discharges, point or multiple point meteorological data; (b) outputs: point (approximately) ambient concentrations
Input Data Requirements	(1) initial set-up and validation: (a) residuals discharges; (b) meteorological data: hourly wind speed, wind direction, mixing heights; (c) several ambient concentration measurements; (d) source coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) CDC 7600; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation; (a) final report available describing theory; (b) user's manual expected to be available soon with data deck format and test case; (3) expertise required: (a) computer programmer; (4) model user qualities: experienced modeler with (a) knowledge of code, diffusion model, photochemistry, and advanced mathematical solution techniques, and (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations of SO_2, NO_x, HC_x, and oxidants; (2) values given at: (a) specified points; (3) format: (a) tabular printout
Costs	(1) model acquisition: (a) model card deck available at no charge from California Air Resources Board, or on a user-supplied magnetic tape; (2) model set-up: program set up and de-bug expected to require several man weeks of effort
Model Accuracy and Sensivity	(1) representativeness to prototype system: (a) extent of description: model has a very simplified one-dimensional air parcel trajectory representation of transport/diffusion processes, model has extremely detailed photochemistry; (b) simplifying assumptions: (a) concentration invariant with height and width (concentration varies with distance), instantaneous mixing through vertical is assumed, state-of-the-art sulfate chemistry requires some assumptions for rate constants; (2) model accuracy: the limited extent and quality of the field test and lack of statistical analysis preclude a quantitative assessment of model accuracy, however it appears that: (a) based upon limited measurements downwind of powerplants to about 10 km., model predictions for ozone seem to be close; (b) for SO_2 and NO_x, up to about 10-15 km. downwind of elevated plant sources, model does not replicate ground-level measured concentrations very well (model predicts highest concentrations at source); (c) amount and quality of field data make it difficult to draw conclusions about accuracy of model sulfate predictions (model predicts highest sulfate concentrations to occur within 10 km. of source); (3) model sensitivity: (a) model sensitive to background concentrations, solar radiation intensity, and spatial and temporal resolution of meteorological data
Other Comments	(1) model limitations/restrictions: (a) "instantaneous" mixing assumption severely limits accuracy of concentration predictions from large point sources within the first 10 km. or so; (b) model does not incorporate residuals discharges which an air parcel "picks up" during its trajectory path; (c) no tests of model predictions seem to have been performed beyond 25 km. from source; (2) special features: (a) model is a modified volumetric model with photochemistry added; (b) models allow for a Gaussian formulation of plume width or another empirical formulation of plume width versus trajectory travel time; (c) wind speed and mixing height may also be input as a function of travel time in order to include spatial and temporal meteorological variations; (d) while model was developed as a trajectory model for large point sources, it could be used with area sources also; (e) model can be used in complex terrain; (3) application experience: (a) model has not been used for analytical studies as yet; (4) pending completion of the user manual, a user may require assistance from model developer (Science Application, Inc.)

Table 5A-27. Summary of the Integrated Model for Plume and Atmospherics in Complex Terrain (IMPACT)

Characteristic	Summary Data
Terrain Characteristics	(1) all types of terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) three options for treatment of photochemical oxidation processes are available: (a) moderately detailed treatment of photochemical reaction formation of ozone and oxidants; (b) a very detailed treatment of photochemical reaction formation of ozone and oxidants; (c) very simple treatment of transformation of SO_2 to sulfates
Mathematical Properties	(1) type of relationship: (a) dynamic; (2) solution methodology: (a) numerically integrated
Time Properties	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) short-term: daily or hourly
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) meso (up to 100 km. or so); (3) discretization: (a) user-specified number of layers (seven were used in tests of elevated powerplant discharges); (b) user-specified number of receptor grids (up to 40 x 20) and grid size; (4) resolution: (a) inputs: point residuals discharge sources, multiple point wind speed and direction, single point inversion height; (b) output: grid area ambient concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point residuals discharges; (b) meteorological data: wind speed and direction, stability class, inversion height; (c) ambient air concentration measurements; (d) source coordinates; (e) receptor coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/168; (b) core storage: 320,000 bytes for typical "non-reactive" problem, 720,000 bytes for typical photochemical problem; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: project report and user's manual available containing: (a) theory; (b) subroutines; (c) data deck format; (d) test case; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with: (a) knowledge of diffusion models, advanced mathematical solution technique, and photochemistry; (b) experience in interpreting model outputs
Output and Output Format	(1) types of output. (a) ambient concentration of SO_2, suspended particulates, NO_x, HC_x, and toxic metals; (2) values given at: (a) grid locations; (3) format: (a) tabular printout; (b) concentration isopleth maps; (4) special features: (a) plot of wind vectors produced by wind field subroutine; (b) table of grid diffusivity coefficients
Costs	(1) model acquisition: (a) model card deck available at no charge from California Air Resources Board, or on a user-supplied magnetic tape;* (2) model set-up: program set-up and de-bug expected to require a few man-months of effort; (3) actual computation: detailed costs not available, but computer runs expected to cost about \$5 to \$6 per simulation hour for nonreactive residuals and \$10 to \$12 per simulation hour and \$25 per simulation hour, respectively, for the simpler and more complex photochemical problem options; total costs, including validation and verification, would run into the tens of thousands of dollars
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: use of grid area resolution for "point" sources can lead to underestimation of ambient concentrations at short distances, SO_2 to sulfate conversion mechanism is rather arbitrary; (b) simplifying assumptions: model does not consider a "sink" term, diffusivity coefficients are assumed equal for x and y directions; (2) model accuracy: (a) initial reported results indicated that predicted hourly concentrations were generally within a factor of 2 for SO_2, NO, and NO_2 in complex terrain during a few days of tests (ozone concentrations were not measured), model developer claims that more recent tests indicate a typical accuracy within 20% for these residuals and O_3; (3) model sensitivity: (a) model predictions were found to be sensitive to the particular diffusivity calculational method, the size of the grid area used, and the quality of the input meteorological data and wind fields
Other Comments	(1) model limitations/restrictions: (a) for point sources there is an important tradeoff between the resolution and accuracy and area extent of calculation; (2) special features: (a) model developers have tried to "piece together" some of the best available submodels for wind fields, diffusivity calculations, plume rise, and photochemistry in order to build IMPACT; (b) a very informative discussion of IMPACT, its submodels, model accuracy and sensitivity is presented in project report and user's guide; (c) although grid model was developed for evaluation of single point sources in complex terrain, multiple point sources and area sources could be evaluated with model; (d) detailed treatment of wind fields and wind shear make model well suited to applications in complex terrain; (3) applications experience: (a) model has been used over complex terrain in Southern California and Arizona; (4) new version of model is available with added features: (a) particle-in-cell option to alleviate point source resolution problem; (b) deposition sink mechanisms; (c) extended sulfate chemistry

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*Alternately, latest model version and support services available for a charge from Form and Substance, Inc., Westlake Village, California.

Table 5A-28. Summary of Reactive Environmental Simulation Model (REM 2)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) photochemical reactions which form ozone from precursors--reactive hydrocarbons and nitrogen oxides--are simulated
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerically integrated, trajectory model
Time Properties	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) short-term: hourly variations in ozone and its precursors, nitrogen oxides and reactive hydrocarbons
Space Properties	(1) dimensionality: (a) two; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) one layer; (b) a 25 x 26 grid is used, each grid element may be 2 miles or 2 kilometers on a side; (c) up to 650 grid area receptors may be specified; (4) resolution: (a) inputs: residuals discharge data as grid areas, point meteorological data; (b) outputs: point ambient concentration calculations
Input Data Requirements	(1) initial set-up and validation: (a) area residuals discharges from mobile and stationary sources, or vehicle and travel data and vehicular emission factors; (b) meteorological data: hourly multiple point wind speed and direction, temperature, dew point, cloud type, mixing height or radiosonde sounding of temperature versus elevation; (e) ambient air concentration measurements--one set for initial conditions and another set for calibration; (f) source grid area coordinates; (g) receptor point coordinates; (2) verification: (a) residuals discharges; (b) meteorological data (see above); (c) two sets of ambient concentration measurements
Computation Status	(1) model status: (a) coded: (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) IBM 370/158 or equivalent; (b) core storage: about 220,000 bytes; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's guide and technical reports which describe: (a) theory; (b) subroutines; (c) data deck format; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with (a) knowledge of code, diffusion model, photochemistry, and advanced mathematical solution techniques, and (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations of O_3, NO, NO_2, HC_x, and CO; (2) values given at: (a) user-specified receptor points; (b) user-specified times; (3) format: (a) tabular printout
Costs	(1) detailed cost estimates are not available: (a) an estimate of the cost of incorporating available activity and residuals discharges inputs would be about $5,000, including about 80 man-days; (b) setting up the computer codes may require a comparable level of effort; (c) clearly the initial costs of model application run into the tens of thousands of dollars and require several months of time; (d) individual computer runs relatively inexpensive, typically about $20 or so (real time to computer time ratio is 600:1)
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model provides an extremely detailed representation of photochemistry, model provides a sparse treatment of atmospheric transport and diffusion processes, residuals discharges/activity information is somewhat less detailed than other models, trajectories may not be responsive to local variations; (b) simplifying assumptions: vertical transport is ignored, vertical diffusion assumes complete mixing through mixing layer, change in wind speed with height is ignored; (2) model accuracy: (a) predicted concentrations for all five residuals were within a factor of 2 or better in three different sized areas in California and Arizona; (3) model sensitivity: (a) model sensitivity has not been reported; (b) model expected to be sensitive to initial concentrations; (c) trajectories sensitive to quality of meteorological wind data
Other Comments	(1) model limitations/restrictions: (a) as a trajectory model, the model must be run repeatedly for each receptor point and time; (2) special features: (a) model has optional subroutines to estimate residuals discharges; (b) trajectories can be run "forward" and "backward" in time; (3) application experience: (a) model has been used in Phoenix, Los Angeles, and Goleta California (three widely varying areas) with very good results for all five residuals

Table 5A-29. Summary of Diffusion Kinetics Model (DIFKIN)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas; (2) code contains a Los Angeles-specific mountain BARRIER subroutine which would have to be altered or removed for other locations
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) photochemical reactions which form ozone from precursors, reactive hydrocarbons and nitrogen oxides, are simulated
Mathematical Processes	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) mathematical: numerically integrated, finite difference
Time Properties:	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) short-term: hourly variations in ozone and its precursors, nitrogen oxides and reactive hydrocarbons
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) multiple layers (user-specified, up to eight); (b) 25 x 25 grid spacing is user-specified; (4) resolution: (a) inputs: residuals discharges as area sources, multiple point wind speed and direction data, multiple point initial concentrations; (b) outputs: ambient concentrations at user-specified receptor points
Input Data Requirements	(1) initial set-up and validation: (a) considerable amount of "stationary" and "mobile" activity data required for model, which generates most residuals discharge data internally; (b) hourly meteorological data at multiple points required to interpolate trajectories; (c) two sets of multiple point ambient concentration measurements: for initial conditions and for calibration; (d) solar angles for day and time
Computation Status	(1) model status: (a) coded, but modifications required for given applications; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) computer type: IBM 360, IBM 370, UNIVAC 1108, or CDC 6400; (b) core storage: 16,000 words; (c) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: user's manual and technical reports together provide: (a) theory; (b) subroutine description; (c) data deck format; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with: (a) knowledge of code, diffusion model, photochemistry, and advanced mathematical solution techniques; (b) experience interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations of ozone, hydrocarbons, nitrogen oxides, and carbon monoxide; (2) values given at: (a) user-specified receptor points; (b) user-specified times; (3) format: (a) tabular printout; (b) punched cards
Costs	(1) while detailed cost estimates are not available, a few users have noted that total costs for initial applications have been around $35,000;[*] about 90% for labor and 10% for computer time; these figures translate to around 500 man-days; (2) it is obvious that many months are required to set up, run, and calibrate the model, in addition to the few months that may be required to develop the residuals discharge data; (3) subsequent applications are estimated typically to cost $15,000 for fairly large urban areas
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: model provides a rather detailed representation of residuals discharges and photochemistry, accuracy of trajectories dependent on quality of meteorological data; (b) simplifying assumptions: horizontal diffusion is ignored, vertical transport is ignored, change in wind speed with height is ignored; (2) model accuracy: (a) in Los Angeles and San Francisco, high correlation coefficients have been found, in Denver correlation was poor; (b) in general model appears to underpredict ozone at low concentrations and overpredict at high concentrations; (3) model sensitivity: (a) model found to be very sensitive to initial "upwind" ambient concentration assumed for the parcel, model quite sensitive to some of the reaction rates and quite insensitive to others
Other Comments	(1) model limitations/restrictions: (a) as a trajectory model, the model must be run repeatedly for each receptor point and time, i.e., model is not necessarily more economical than a "fixed grid" model; (b) a few changes in model are required to apply model for cities other than Los Angeles; (c) specialized expertise required to use model; (2) special features: (a) model includes "separable" detailed subroutines to generate most of the residuals discharge information needed in models; (b) comparatively good information has been published about the strengths and weaknesses of the model (see annotated bibliography); (c) trajectories can be run "forward" and "backward" in time; (3) application experience: (a) model use has included applications in Los Angeles San Francisco, Denver, Las Vegas, and Reno; (4) new version of DIFKIN has been developed at Environmental Research & Technology, Santa Barbara, California with: (a) expanded photochemical mechanism; (b) treatment of wind shear effects; (c) new numerical integration method, and (d) new submodel for residuals discharges

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[*] See Record, F.A., et al., "Photochemical Oxidant Modeling: Volume I - Techniques Applicable to Highway System Evaluation," EPA-450/3-75-069a, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, July 1975.

Table 5A-30. Summary of Systems Applications, Inc. Photochemical Model (SAI)

Characteristic	Summary Data
Terrain Characteristics	(1) urban areas and all types of terrain
Physical Processes	(1) transport and diffusion
Chemical Processes	(1) photochemical oxidation reactions; (2) dry deposition
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) numerically integrated, finite difference
Time Properties	(1) time variability of inputs: (a) dynamic; (2) time period of outputs: (a) short-term: daytime buildup of photochemical oxidants and precursors, hourly variations in ozone and precursors
Space Properties	(1) dimensionality: (a) three; (2) spatial scale of application: (a) micro; (b) meso; (3) discretization: (a) multiple layers (user-specified); (b) 25 x 25 grid spacing is user-specified; (4) resolution: (a) inputs: residuals discharges as area and point sources, multiple point wind speed, direction, and mixing height data, multiple point ambient concentration; (b) outputs: area grid concentrations
Input Data Requirements	(1) initial set-up and validation: (a) activity data and residuals discharge data for point and area sources; (b) hourly meteorological data at multiple points: wind speed, wind direction, mixing heights, ambient temperature; (c) two sets of ambient concentration measurements; (d) source and receptor grid coordinates; (2) verification: (a) residuals discharge data; (b) meteorological data (see above); (c) ambient concentration measurements
Computation Status	(1) model status: (a) coded; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) CDC 7600, UNIVAC 1100, or equivalent; (b) program language: FORTRAN IV
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency and private agency (see annotated bibliography); (b) model available for general use; (2) availability of model documentation: (a) user's guide and system manual available from NTIS; (3) expertise required: (a) computer programmer; (b) research assistant; (4) model user qualities: experienced modeler with: (a) knowledge of code, diffusion model, photochemistry, and advanced mathematical solution techniques; (b) experience in interpreting model outputs
Output and Output Format	(1) types of output: (a) ambient concentration of NO_x, HC_x, CO, and oxidants; (2) values given at: (a) grid areas; (b) interpolated points; (3) format: (a) printed hourly-averaged ground and upper level concentration maps; (b) printed summary of hourly-averaged vertical concentration distribution at each monitoring station; (c) printed hourly-averaged ground level map of concentration variations from each grid cell; (d) printed instantaneous ground and upper-level concentration maps; (e) printed summary of instantaneous vertical concentration distribution above each monitoring station.
Costs	(1) not possible to specify detailed costs at present time; however, total cost of initial application expected to be $30,000 to $70,000 with subsequent computer time cost of several hundred dollars per run
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: input variations in wind speed and direction add realism, fixed horizontal diffusion coefficient detracts from actuality; (2) model accuracy: (a) limited application makes the assessment difficult at present; (3) model sensitivity: (a) known to be sensitive to residuals discharges, initial conditions and boundary conditions, and reaction rates
Other Comments	(1) model limitations/restrictions: (a) model application limited by complexity of data requirements; (b) modifications required to eliminate "site-specific" features; (2) special features: (a) model has subroutine which generates residuals discharges; (b) model is actually a combined activity and air quality model; (c) model provides a detailed treatment of both chemical reactions and area-wide meteorological conditions; (3) application experience: (a) model has been applied to Los Angeles, Denver, and Turin, Italy; (4) new version of model will be available in July 1978 containing several changes: (a) fully three-dimensional wind inputs; (b) algorithms for generating the wind inputs; (c) new diffusivity scheme that incorporates the effects of surface roughness and atmospheric stability; (d) a 42-step reaction mechanism to describe ozone formation, SO_2 oxidation, and aerosol formation; (e) the capability to treat SO_2 and aerosols; (f) removal of residuals using the deposition velocity concept; (g) microscale module to treat the reaction of NO emitted from roadways with ambient O_3; (h) an improved numerical integration technique; (i) a complete revision of the computer codes to make them more readily implementable on different computers

Table 5A-31. Summary of Nonlinear Rollback Appendix J Model (Appendix J)

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) transport and diffusion not explicitly modeled
Chemical Processes	(1) photochemical reactions not explicitly modeled
Mathematical Properties	(1) type of relationship: (a) deterministic
Time Properties	(1) time variability of inputs not explicitly considered; (2) time period of outputs: (a) short-term: hourly
Space Properties	(1) spatial scale of application: (a) meso; (2) resolution: (a) inputs: changes in urban area residuals discharges assumed to apply proportionately to existing spatial pattern; (b) outputs: ambient concentration estimates at receptor points
Input Data Requirements	(1) rollback: (a) ambient concentration measurements--generally hydrocarbons and oxidant/ozone--to determine nonlinear relationship; (2) rollforward: (a) ambient concentration measurements; (b) projected changes in residuals discharges
Computation Status	(1) model uncoded; (2) equipment needed: none
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) availability of model documentation: see annotated bibliography; (3) expertise required: (a) no specific job positions required; (4) model user qualities: (a) understanding of model principle and limitations
Output and Output Format	(1) types of output: (a) rollback: reductions in residuals discharges; (b) rollforward: ambient concentration
Costs	(1) rollback/rollforward model itself can be developed within a few man-days from ambient monitoring data
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) extent of description: changing spatial and temporal patterns of residuals discharges are not considered, ozone/oxidant treated as a function of hydrocarbons only; (b) simplifying assumptions: same meteorological conditions as for base case, unchanging spatial and temporal residuals discharge distributions; (2) model accuracy: "first cut," rough approximation only
Other Comments	(1) model limitations/restrictions: (a) rollback/rollforward models consider only the relationship between ozone/oxidants and a single precursor hydrocarbon, model cannot consider combined changes in hydrocarbons and nitrogen oxides; (b) rollforward model is of questionable value in projecting ambient oxidant/ozone changes from site-specific projects; (2) special features: (a) rollback and rollforward models can best be used to study "area-wide" strategies or changes such as vehicular discharge limitations, number of automobiles, vehicle miles traveled projections; (b) rollback and rollforward models might be used as a "screening technique" to decide which strategies to evaluate further in a spatial and temporal photochemical model; (c) several variations of model are possible: the nonlinear relationships can be developed for specific cities and specific monitoring locations within city, or national appendix J relationship could be used, or relationships could be developed for both hydrocarbons and nitrogen oxides

Note: Model can be used for preliminary analysis.

Table 5A-32. Summary of Croke-Roberts Model

Characteristic	Summary Data
Terrain Characteristics	(1) all terrain types
Physical Processes	(1) none explicitly modeled
Chemical Processes	(1) none
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) statistical: regression
Time Properties	(1) time variability of inputs: (a) steady-state; (b) quasi-steady-state; (c) dynamic; (2) time period of outputs: (a) short-term: few hours or less; (b) long-term: seasonal, annual average
Space Properties	(1) dimensionality: not applicable; (2) spatial scale of application: (a) micro; (b) meso; (c) macro; (3) discretization: (a) user-specified number of grids; (b) user-specified number of receptors; (4) resolution: (a) inputs: residuals discharge data as point or area sources; (b) outputs: point concentrations
Input Data Requirements	(1) initial set-up and validation: (a) point and area residuals discharges; (b) numerous ambient air concentration measurements; (2) verification: (a) point and area residuals discharges; (b) numerous ambient air concentration measurements
Computation Status	(1) model status: (a) uncoded, but can be used with readily available computer programs; (2) equipment needed: (a) digital computer; (b) hand calculator for "small" problems
Output and Output Format	(1) types of output: ambient concentration; (2) values given at: ambient monitoring (receptor) points
Ease of Application and Manpower Needs	(1) availability of model documentation: (a) no formal documentation exists, but some information from authors and articles (see annotated bibliography); (2) expertise required: (a) no formal job positions required; (3) model user qualities: (a) mathematical ability through algebra and statistics; (b) understanding of model principles and limitations; (c) experience in interpretation of model outputs, or access to consultations
Costs	(1) data preparation: (a) for "short-term" problems which require sorting of seasonal data several days may be required; (b) for "long-term" problems less effort required; (2) actual computation: (a) dependent upon number of sources and receptors, hand calculations can be done in a couple of man-days and computer calculations at very nominal expense; (3) output analysis: (a) analysis of results: varies with problem, but routine validation or verification can be done in five man-days
Model Accuracy and Sensitivity	(1) representativeness to prototype system: (a) model does not attempt to describe system and cause/effect relationships; (2) model accuracy: (a) accuracy can vary widely from receptor point to point or problem to problem; (3) model sensitivity: (a) sensitive to residuals discharge errors, relative sensitivity to different discharges can be determined
Other Comments	(1) model limitations/restrictions: (a) analysis of changes in spatial patterns of residuals discharge is difficult or impossible; (b) analysis of stack height changes not possible; (c) applicability restricted by ambient monitoring data availability; (d) defining and setting up problem properly can be difficult; (2) special features: (a) model can be applied in all terrain conditions

Note: Model can also be used for preliminary analysis.

Table 5A-33. Summary of Repro Model

Characteristic	Summary Data
Terrain Characteristics	(1) "rough" urban areas
Physical Processes	(1) not applicable to repro model, applicable to original model
Chemical Processes	(1) not applicable to repro model, applicable to original model
Mathematical Properties	(1) type of relationship: (a) deterministic; (2) solution methodology: (a) statistical: multi-variate curve fitting (piecewise linear)
Time Properties	(1) time variability of inputs: (a) dynamic (as original model); (2) time period of outputs: (a) short-term: several hours or less
Space Properties	(1) not applicable to repro model, applicable to original model
Input Data Requirements	(1) residuals discharges, as a percentage "base case" condition: (a) mobile source NO_x discharges; (b) mobile source hydrocarbon discharges; (c) fixed source hydrocarbon discharges; (2) initial ambient concentrations: (a) NO_x; (b) hydrocarbons; (3) selected ambient concentration calculations from original model
Computation Status	(1) model status: (a) coded for specific application to Los Angeles; (2) equipment needed: (a) digital computer; (3) computer characteristics: (a) CDC 6400
Ease of Application and Manpower Needs	(1) availability of operational model and supporting information: (a) public agency; (2) available model documentation includes: (a) theory; (b) subroutines; (3) expertise required: (a) computer programmer; (b) experienced modeler with knowledge of multivariate methods to develop repro model and specialized expertise to use the original photochemical model--such as the SAI model--on which repro model is based; (4) model user qualitities: (a) understanding of model principles and limitations; (b) experience in interpretation of model outputs
Output and Output Format	(1) types of output: (a) ambient concentrations; (2) values given at: (a) user-selected points; (3) format: (a) tabular printout
Costs	(1) cost of setting up original model will run into the tens of thousands of dollars for applications outside Los Angeles, unless use of original photochemical model is available from other users; (2) cost of running original model to obtain the relations (for the repro model) between ambient concentration and residuals discharges could run into the thousands, or tens of thousands of dollars; (3) cost of setting-up statistical repro model would involve several man-weeks of effort
Model Accuracy and Sensitivity	(1) model accuracy: repro model is as accurate as original model it "models;" (2) model sensitivity: (a) ozone concentrations were affected more by hydrocarbons discharges than by NO_x discharges; (b) initial concentrations have a major effect upon predicted air quality; (c) sensitivity of ozone concentration to changes in NO_x discharges varies with ozone concentration levels
Other Comments	(1) model limitations/restrictions: (a) use of repro model dependent upon availability of original model; (b) use of repro model is restricted to study only a limited number of input and output variables of original model; (c) changes in spatial locations of discharges cannot be modeled and meteorological conditions are assumed to be the same for the base case; (2) special features: (a) repro model actually models the original model by developing statistical relations between selected inputs and outputs of original model; (b) after repro model is operational, computing time is exceedingly fast: milliseconds versus tens of minutes for original model; (c) unfortunately this advantage seems to be self-defeating for most applications since the development of the repro model required 100 runs of the more expensive model*

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*Based upon the single reported application to Los Angeles.

Appendix B

ANNOTATED BIBLIOGRAPHY FOR AIR QUALITY MODELS

Gifford-Hanna Model

Gifford, F. A. 1973. The Simple ATDL Air Pollution Model, revised, ATDL Contribution File No. 78 (Oak Ridge, Tennessee, National Oceanic and Atmospheric Administration Atmospheric and Diffusion Laboratory).

Paper describes the conceptual and mathematical basis of the Gifford-Hanna model and simplifying assumptions. The author demonstrates that for the urban discharge patterns a simple diffusion model for area sources is appropriate. Comparisons of the ATDL and other models are given for several cities with respect to correlation coefficient between observed and calculated concentrations.

Gifford-Hanna Photochemical Model

Record, F. A., R. M. Patterson, D. A. Bryant, and A. H. Castaline. 1975. Photochemical Oxidant Modeling, Vol. I: Techniques Applicable to Highway System Evaluation, Publication No. EPA-450/3/75-069a (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

A brief technical description is given for the Gifford-Hanna Photochemical Model (and several other models). Based on some comparisons of predicted versus observed concentrations, the model applicability and reliability are analyzed. The data requirements, manpower requirements and limitations, and special features are also discussed.

Hanna, S. R. 1973. "A Simple Dispersion Model for the Analysis of Chemically Reactive Pollutants," Atmospheric Environment vol. 7, pp. 803-817.

The basic Gifford-Hanna model is reviewed. A technical discussion of the theory and derivation of a steady-state solution to a set of photochemical reactions as the basis of the photochemical model is presented. An application of the Gifford-Hanna Photochemical Model to Los Angeles is described and compared with another model.

Air Quality Display Model

National Air Pollution Control Administration. 1969. *Air Quality Display Model (User's Manual)* (Washington, D.C., National Air Pollution Control Administration) and available as NTIS Publication No. PB 189-194.

As the basic manual for the Air Quality Display Model, this document contains a discussion of the computer program, its subroutine, the preparation of data inputs, and data formats. The basic theory and Gaussian equations of the model are also discussed. A test case for setting up the model is presented, along with examples of model outputs. A complete card listing along with flow diagrams of subroutine is included.

Climatological Dispersion Model

U.S. Environmental Protection Agency. 1973. *User's Guide for the Climatological Dispersion Model*, Publication No. EPA-450/3-77-015 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This basic manual for the use of the Climatological Dispersion Model discusses the computer program, including subroutines, preparation of data inputs and data formats. The theory and adaptation of the Gaussian model equations are given. A test case for setting up the model, along with examples of model outputs, is given. A complete card listing is presented, as is a flow diagram.

U.S. Environmental Protection Agency. 1977. *Addendum to User's Guide for the Climatological Dispersion Model*, Publication No. EPA-450/3-77-015 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This guide supplements the original *User's Guide for the Climatological Dispersion Model* by discussing the new features of the revised CDM, called CDMQC. These features discussed include (1) a source contribution table, (2) a statistical calibration subroutine, and (3) a statistical conversion of averaging times using the Larsen model. The new CDMQC computer code is discussed, including data inputs and data formats, and model outputs. An expanded test case is presented, along with a model card listing.

Transportation and Air Shed Simulation Model

U.S. Department of Transportation. 1974a. *TASSIM: A Transportation and Air Shed Simulation Model. Vol. I. Case Study of the Boston Region* (Washington, D.C., U.S. Department of Transportation) and available as NTIS Publication No. PB 232-933.

A brief description of the model and submodel is given, but the main emphasis is on the use of the TASSIM Model for policy simulation in the Boston region. Several alternative transportation policies are analyzed for their impacts upon ambient air quality and the cost effectiveness of different policies. In the context of the Boston application, certain limitations of the model are analyzed.

U.S. Department of Transportation. 1974b. TASSIM: A Transportation and Air Shed Simulation Model. Vol. II. Program User's Guide (Washington, D.C., U.S. Department of Transportation) and available as NTIS Publication No. PB 232-934.

This document is the basic manual for the use of TASSIM and the three submodels: the transportation traffic flow submodel, the transportation source discharge submodel, and the atmospheric diffusion submodel. The respective subroutines of the respective submodels are discussed, including data inputs. A card listing of the complete TASSIM programs is given.

COPOLLUT

Department of Transportation, State of Ohio. COPOLLUT User's Manual (Columbus, Ohio, Ohio Department of Transportation).

This user's manual describes the two subroutines of the COPOLLUT Model. The first subroutine develops temporal and spatial patterns of link and mode traffic source discharges from inputs of historical traffic volume and vehicle speed data. The second subroutine performs diffusion calculations for the highway and adjacent receptor points. Data inputs and formats are discussed.

California Line Source Dispersion Model

Ward, C. E., Jr., A. J. Ranzieri, and E. C. Shirley. 1976. CALINE 2--An Improved Microscale Model for the Diffusion of Air Pollutants from a Line Source (Sacramento, Calif., California Department of Transportation).

Report serves as complete documentation of CALINE 2 Model. The Gaussian model theory and assumptions are reviewed, as well as the line source model's treatment of various special cases of source/receptor geometries. A discussion of data inputs and formats is presented, as well as a card listing of the model (in an appendix). In addition, typical model applications are discussed, along with completed model verification and model sensitivity tests.

EPA HIWAY

U.S. Environmental Protection Agency. 1974. User's Network for Applied Modeling of Air Pollution (UNAMAP) (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency) and available as NTIS Publication No. PB 229-777.

Document describes basic UNAMAP series of models, including HIWAY. Basic documentation which describes model formulation, subroutines, data inputs and outputs.

Point, Area, and Line Source Model

Turner, B. D. and W. B. Petersen. 1975. "A Gaussian-Plume Algorithm for Point, Area, and Line Sources," Paper presented at 6th NATO/CCMS International Technical Meeting on Air Pollution Modeling (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency, September).

Paper describes the calculational algorithm and equations employed in the PAL Model for microscale air quality impacts of point, area, and line sources. Particular attention is given to how the algorithm models the complicated source-receptor geometries and uses numerical integration of the Gaussian point source equation. Data requirements, including the detailed sources coordinates required, are also noted for several problem contexts.

Single Source Model (CRSTER)

U.S. Environmental Protection Agency. 1977. User's Manual for the Single Source (CRSTER) Model, Publication No. EPA-450/2-77-013 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

Thorough documentation for the CRSTER Model is given. A discussion of the Gaussian plume equations used, basic assumptions, and conceptual approach of the CRSTER Model formulation (with respect to terrain consideration) are given. The various subroutines, including the preprocessor program which massages input data into desired variables, are discussed, and a card listing is given. A test case demonstrating program inputs and outputs is presented. Several additional aspects, including model applications, model validation, and model sensitivity, are discussed in appendices.

APRAC 1A

Mancuso, R. L. and F. L. Ludwig. 1972. User's Manual for APRAC 1A Diffusion Model Computer Program (Menlo Park, Calif., Stanford University Research Institute).

Documentation describes the respective basic subroutines which (1) estimate transportation source discharge from traffic flow input data, and (2) estimate ambient carbon monoxide concentrations from a Gaussian diffusion model. The street canyon model for localized concentrations is presented. Required data inputs, transportation network grids, and spatial source aggregation are discussed.

Ludwig, F. L. and W. F. Dabberdt. 1972. Evaluation of the APRAC 1A Diffusion Model for Carbon Monoxide (Menlo Park, Calif., Stanford University Research Institute) and available as NTIS Publication No. PB 210-819.

This report describes detailed field studies performed in the St. Louis area in order to test both the source discharge and the street canyon diffusion submodels, and presents the results of the studies. The equipment used, sampling patterns, and measurements taken in the program are discussed in detail and the submodels are evaluated.

PTMAX

See EPA HIWAY, above.

PTDIS

See EPA HIWAY, above.

PTMTP

Guzewich, D. C. and J. B. Pringle. 1977. "Validation of the EPA-PTMTP Short-Term Gaussian Dispersion Model," Journal of the Air Pollution Control Association vol. 27, no. 6, pp. 540-542.

This article describes the field experiments and results of a gaseous dispersion tracer study undertaken at the Rocky Mountain Arsenal in order to validate the PTMTP model downwind of a single point source. The stability class determination required for the model calculation was determined in three different ways: wind fluctuation measurements, temperature difference measurements, and the Pasquill-Turner surface observations; stability classification was found to be the major cause of discrepancies between measured and calculated concentrations.

See also EPA HIWAY, above.

Real Time Air Pollution Model

Novak, J. H. and B. D. Turner. 1976. "An Efficient Gaussian-Plume Multiple-Source Air Quality Algorithm," Journal of the Air Pollution Control Association vol. 26, no. 6, pp. 570-575.

Paper describes the conceptual basis of the RAM Gaussian diffusion model for point and area sources and the one-dimensional numerical integration technique employed. Basic point and area source and meteorological data inputs are described. User options for specifying point and area source and reception locations are presented.

Gaussian Evaluation Model

Fabrick, A. J., R. C. Sklarew, and J. C. Wilson. 1977a. Point Source Model Development Study, prepared for the California Air Resources Board (Westlake Village, Calif., Science Applications, Inc.).

Report discusses and illustrates the technical approaches used in the GEM for the respective subroutines. Along with the basic Gaussian model, a discussion of how the model is modified for diffusion parameters and plume trajectories in complex terrain is presented. The model options for plume rise formula and diffusion parameter curves are also discussed.

__________, __________, and __________. 1977b. Point Source Model Development Study. Appendix A. User's Guide to GEM, prepared for the California Air Resources Board (Westlake Village, Calif., Science Applications, Inc.).

Along with briefly summarizing the technical approaches and calculational formulae presented in the above report, this document serves as the basic user's manual. The program subroutines are discussed and subroutine inputs and outputs are specified. Data deck formats and a sample test case with data inputs and model outputs are presented. A computer program listing is given.

Argonne Puff Model

Roberts, J. J., E. J. Croke, A. S. Kennedy, J. E. Norco, and L. A. Conley. 1970. A Multiple-Source Urban Atmospheric Dispersion Model, ANL/ES-CC-007 (Argonne, Illinois, Argonne National Laboratory).

This report discusses the theory of the Argonne Puff Model, describes the model's calculational approaches, the computer code subroutines, and model validation study. Model input requirements and the area source and receptor grids are discussed. A listing of the model subroutines is given.

Stanford Research Institute

Ruff, R. E., F. L. Ludwig, L. S. Gasiorek, A. Chaplin, W. S. Meisel, S. Miller, and H. J. Payne. Design Manual for an SO_2 Emission Limitation Program for the Kingston Steam Plant, Vols. I and II, prepared for the Tennessee Valley Authority, Muscle Shoals, Alabama (Menlo Park, Calif., Stanford Research Institute).

Volume I primarily describes the formulation of the puff model and the real time model forecast of concentrations predictions downwind of the TVA Kingston plant. The basic puff model theory and calculation of the puff diffusion parameters are discussed. Volume II describes the different program subroutines (with detailed flow charts) and gives a program card listing.

GLUMP

Lyons, W. Great Lakes Mesometeorological Project, Report prepared for U.S. Environmental Protection Agency, Division of Meteorology, Research Triangle Park, North Carolina (Milwaukee, Wisconsin, University of Wisconsin).

Research report describes the Gaussian diffusion model developed for application in coastal regimes; model allows for the input of a variable mixing layer height with distance for shoreline. The field investigations undertaken in support of the model development are also discussed.

VALLEY

Burt, E. W. 1977. VALLEY Model User's Guide, Publication No. EPA-450/2-77-018 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

User's guide discusses the Gaussian diffusion equation and special features of plume trajectories used to represent complex terrain. Application of the model to 24 hour and long-term periods is discussed. Detailed comments are given on the model limitations and applications are presented. The model data requirements and data deck format are discussed. Appendices include a test case of model inputs and outputs, a computer card listing of the model, and a validation study of the model.

Oak Ridge Fog and Drift Model

LaVerne, M. E. 1977. The Oak Ridge Fog and Drift Code (ORFAD) User's Manual, ORNL/TM-5201 (Oak Ridge, Tennessee, Oak Ridge National Laboratory, Energy Division).

The mathematical modeling of the physical processes is presented for plume rise, fog formation, drift deposition (and evaporation) as a function of relative humidity. In addition to the discussion of required data inputs and card deck formats, certain optional inputs and override features of the computer code are given. Listings of representative tabular and graphical outputs are given, in addition to the program card listing.

Atmospheric Transport Model

Culkowski, W. M. and M. R. Patterson. 1976. A Comprehensive Atmospheric Transport and Diffusion Model, ORNL/NSF/EATC-17 (Oak Ridge, Tennessee, Oak Ridge National Laboratory).

The basic documentation for the Atmospheric Transport Model discusses the various physical processes modeled and their mathematical representations, including dry deposition, gravitational settling, wet deposition, and resuspension, in addition to the Gaussian transport and diffusion. The data inputs are enumerated and discussed; a sample problem illustrates the data inputs and model outputs. The computer card listing is presented as an appendix. A comprehensive set of references for deposition problems is included.

Drift Transport Cooling Tower

Webb, R. O., G. O. Schrecker, and D. H. Guild. Drift from the Chalk Point Natural Draft Brackish Water Cooling Tower: Source Definition, Downwind Measurements, and Transport Model, prepared for the State of Maryland Power Plant Siting Program, Chalk Point Cooling Tower Project (Knoxville, Tennessee, Environmental Systems Corporation).

Report describes a field validation measurement program of drift droplet mass fraction discharges, and the ground level salt concentration and deposition predicted by the Drift Transport Cooling Tower Model. The model is described with respect to the gravitational settling, evaporation, and diffusion processes incorporated into the Gaussian model. Limited test results are presented comparing the model and another drift model with measured ambient concentration and deposition.

The Research Corporation of New England Cooling Systems Model

Davis, E. L., C. R. Case, G. F. Collins, and E. A. Pearson. 1974. An Evaluation of Potential Atmospheric Impact of Alternative Cooling Systems for the Erie Nuclear Plant (Wethersfield, Conn., The Research Corporation of New England).

Document describes the frequency of fog projected to occur under specified plant and cooling tower operating conditions for representative area meteorological conditions. TRC Fog Model is described, the basic Gaussian equation is used to predict water evaporation concentrations in order to determine if the added vapor plus natural background water vapor will result in fog condensation.

Texas Episodic Model

Christiansen, J. H. 1976. "Design and Application of the Texas Episodic Model," in Proceedings of the EPA Conference on Environmental Modeling and Simulation, Publication No. EPA-600/9-76-016 (Cincinnati, Ohio, U.S. Environmental Protection Agency).

This paper is a synopsis of the material presented in the User's Guide to the Texas Episodic Model (which also contains the computer program listing). The "short-term" Gaussian model point source equation and the Gifford-Hanna area source equations are discussed, and the calculational shortcuts employed are discussed. The model inputs and outputs and user options are explained. Several examples of the model use for practical air quality problems are given. The calculational advantages of the Texas Episodic Model are illustrated.

International Business Machines Air Quality Model

Shir, C. C. and L. J. Shieh. 1975. Development of Urban Air Quality Simulation Model with Compatible RAPS Data, Publication No. EPA-600/4-75-005a (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

A discussion of the model development objectives in conjunction with the EPA St. Louis RAPS study is given. The model formulation, including grid options, numerical equations, boundary conditions, initial conditions, diffusivity coefficient, and wind fields is discussed. The computer model subroutines and their functions and input specifications and requirements are given. An auxiliary program used to process residuals discharge source data is also discussed.

INTERA

Lantz, R. B., G. F. Hoffnagle, and S. B. Pahwa. 1976. "Diffusion Model Comparisons to Measured Data in Complex Terrain," Paper presented at Third Symposium on Atmospheric Turbulence and Diffusion, Raleigh, North Carolina (Boston, Mass., American Meteorological Society).

Because the INTERA numerical model was developed for application in complex terrain, this paper discusses three field trace validation studies in mountainous areas. The INTERA model and two other models are compared for their predictive abilities. The advantages of using the numerical model with a complex localized wind field are underscored in the test results.

Atmospheric Particle-in-Cell Model

Lange, R. and C. Sherman. 1977. "Particle-in-Cell Vs. Straight Line Gaussian Calculations for an Area of Complex Topography," Paper presented at Joint Conference on Applications of Air Pollution Meteorology, Salt Lake City, Utah, sponsored by the American Meteorological Society and the Air Pollution Control Association (Boston, Mass., American Meteorological Society).

Paper describes the ADPIC code and the various processes simulated, including wet and dry deposition, gravitational settling, and decay. A submodel, MATHEW, which provides the wind field to ADPIC, is also described. Various field validation studies are mentioned, but a comparison of the results from ADPIC and a Gaussian Diffusion in the Hudson River Valley is discussed in detail.

Scavenging Model Incorporating Chemical Kinetics

Dana, M. T., D. R. Drewes, D. W. Glover, and J. M. Hales. 1976. Precipitation Scavenging of Fossil Fuel Effluents, Publication No. EPA-600/4-76-031 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This interim research report discusses the SMICK model for precipitation scavenging of reactive pollutants from power plant plumes. The droplet collection, liquid-phase chemical reaction, and desorption of residuals are discussed and described mathematically. The field experiments taken at a stream electric plant are discussed, and results with respect to the variation of scavenging with distance and different residuals are presented.

Atmospheric Carbon Monoxide Transport Model

Carlson, R. and W. Norton. 1976. User's Guide for Carbon Monoxide Transport Model (Fairbanks, Alaska, Institute of Water Resources) and available as NTIS Publication No. PB 259-719.

This documentation report provides a detailed conceptual and mathematical description of the numerical model and its finite element solution technique; several examples of problems and the way to structure and solve them are presented. Required data inputs and card formats are explained, along with model options. Each subroutine and its function is described. An appendix contains a tabular listing of model inputs and outputs for use as a test problem.

Livermore Regional Air Quality Models I and II

MacCracken, M. C. and G. D. Sauters, eds. 1975. Development of an Air Pollution Model for the San Francisco Bay Area, Final Report to the National Science Foundation (Livermore, Calif., Lawrence Livermore Laboratory).

This report contains both summaries and detailed descriptions of the technical development of the LIRAQ I (nonreactive) and LIRAQ II (photochemically reactive) models. The numerical solution methodology required, meteorological data inputs and the development and wind fields are discussed. The development of the photochemical reaction scheme used in LIRAQ II is described in detail. The model verification program and results are presented. Finally, several examples of the use of the LIRAQ models in air quality management contexts are given.

__________. 1975. User's Guide to the LIRAQ Model for the San Francisco Bay Area (Livermore, Calif., Lawrence Livermore Laboratory).

This user's guide complements the above report for both LIRAQ I and II. Although brief descriptions of the model technical approaches are given, this document primarily serves to describe the computer program, its subroutines, data inputs and formats, model grid system and base maps, and model options. The actual computer program listing is included on microfiche.

Reactive Plume Model

Liu, M-K., D. Durran, P. Mundkur, M. Yorke, and J. Ames. 1976. Final Report. The Chemistry, Dispersion, and Transport of Air Pollutants from Fossil Fuel Power Plants in California: Data Analysis and Emission Impact Model, prepared for the California Air Resources Board, Sacramento, California (San Rafael, Calif., Systems Applications, Inc.).

This report describes the development of the Reactive Plume Model. A simple mass balance approach is developed to describe ambient concentration along the plume trajectory. The chemical reaction mechanism and numerical solution technique are discussed. Field validation studies for the model as conducted on several different days in several different locations for the residuals of interest are presented.

Chemically Reactive Power Plant Plume Model

Miksad, R. W., K. K. DeBowers, and J. R. Brock. 1977. "A Chemically Reactive Power Plant Plume Model" (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency, Aerosol Research Branch, Environmental Sciences Research Laboratory).

Paper addresses the modeling of photochemically reactive residuals in a power plant plume. The problem is subdivided into two stages: a diffusion problem and a chemically reactive problem which is solved independently. A Gaussian diffusion solution is used; results of model predictions are then compared with ambient plume measurements over several distances downwind of the power plant.

Integrated Model for Plume and Atmospherics in Complex Terrain

Fabrick, A. J., R. C. Sklarew, and J. C. Wilson. 1977. Point Source Model Evaluation and Development Study, prepared for the California Air Resources Board, Sacramento, California (Westlake Village, Calif., Science Applications, Inc.).

Report describes the several options that were considered for the wind field submodel, diffusivity coefficient submodel, and photochemical submodel, and why particular options were chosen. Then a detailed discussion of the model field validation undertaken on various days at different locations in complex terrain is given for the respective residuals. This report is intended for use in conjunction with the User's Guide attached as Appendix C of the report. The User's Guide describes the subroutines, data input requirements, and formats. Sample program outputs are provided.

Sklarew, R. C., J. C. Wilson, and A. J. Fabrick. 1977. "DEPICT/IMPACT Grid Models of Reactive Point Source Emissions in Complex Terrain," Paper presented at Joint Conference on Applications of Air Pollution Meteorology, Salt Lake City, Utah, sponsored by the American Meteorological Society and the Air Pollution Control Association (Boston, Mass., American Meteorological Society).

Paper primarily describes the application of IMPACT to complex terrain diffusion problems. In particular, the wind field subroutine is shown to provide good representation of the plume transport. The observed and predicted concentrations are compared for time periods of two different sites.

Brookhaven National Laboratory Long and Short Range Air Quality Model

Meyers, R. E., R. T. Cederwall, and J. A. Storch. 1978. "Atmospheric Pollution from Fossil Fuel Energy: Risk Impact Analysis," in Final Report of Committee on Nuclear and Alternative Energy Systems (Washington, D.C., National Academy of Sciences).

This report describes the basic numerical trajectory model developed at Brookhaven, including the incorporation of dry and wet deposition, and chemical decay and transformation into the basic equation. Field validation study results for SO_2 and sulfates are presented and a rather detailed discussion of model sensitivity is given. Report also discusses the public health impact assessment from air quality as undertaken by Brookhaven.

Statistical Turbulent Incompressible Fluid Flow Model

Taft, J. 1974. A Numerical Model for the Investigation of Most Buoyant Cooling Tower Plumes (La Jolla, Calif., Systems, Science and Software).

This report describes a basic hydrodynamics model in which equations expressing conservation of mass, energy, momentum, and moisture are solved numerically; in particular, the ambient moisture concentration determines the presence or absence of fog. Some plume observations taken in the vicinity of the Keystone power plant are compared with predictions.

Westinghouse Cooling Tower Model

Roffman, A. and R. Grimble. 1974. "Drift Deposition Rates from Wet Cooling Systems," Paper presented at Symposium on Cooling Tower Environments, The University of Maryland, College Park, Maryland, March 4-6.

This paper describes the Westinghouse model for drift deposition calculations. The numerical model includes changes in droplet concentration due to evaporation and condensation in conjunction with the conservation of mass equation. Calculations are performed for representative cooling systems (spray canals, mechanical draft towers, and natural draft towers) under given meteorological conditions and the spatial distribution of drift deposition is compared.

Reactive Environment Simulation Model

Kokin, A., L. G. Wayne, and M. Weisbur. 1973. Controlled Evaluation of the Reactive Environmental Simulation Model Guide (REM). Volume II: User's Guide (Santa Monica, Calif., Pacific Environmental Sciences Service) and available as NTIS Publication No. PB 220-457.

This report describes the design, operation, and use of the original REM numerical model. The technical analysis performed by each subroutine is explained and illustrated by flow charts. The program input and card deck format is presented and a program card listing is given. The guide also includes a conceptual diagram and discussion of photochemical modeling in general.

Drivas, P. J., M. Chan, and L. G. Wayne. 1977. "Validation of an Improved Photochemical Air Quality Simulation Model," Paper presented at Joint Conference on Applications of Air Pollution Meteorology, sponsored by American Meteorological Society and Air Pollution Control Association (Boston, Mass., American Meteorological Society).

This paper describes some of the model improvements incorporated into REM 2, the new version of REM. Model assumptions are stated and the revised photochemical mechanism is discussed. The paper presents the results for validation studies for five residuals in three different-sized cities with varying terrain features.

Diffusion Kinetics Model

Martinez, J. R., R. A. Nordsieck, and M. A. Hirschberg. 1973. User's Guide to Diffusion Kinetics Code, Publication No. EPA-R4-73-012 vol. b (Santa Barbara, Calif., General Research Corporation).

User's guide describes the technical modeling approach, equations, and the model assumptions. Data inputs and formats are explained and illustrated. The respective functions of each subroutine are explained and illustrated.

Record, F. A., R. M. Patterson, M. T. Mills, E. P. V. Ward, D. A. Bryant, and B. B. Galkiewicz. 1975. Photochemical Oxidant Modeling. Vol. II. Detailed Technical Report, Publication No. EPA-450/3-75-069b (Bedford, Mass., GCA Technology Division).

This report contains a detailed evaluation of the DIFKIN model, which was developed in Los Angeles, for a model application to Denver. Required computer program modifications are discussed, and the most important data inputs are highlighted. Predicted model concentrations for several wind trajectories were compared with ambient measured concentrations.

Center for the Environment and Man

Pandolfo, J. B., C. A. Jacobs, R. J. Ball, M. A. Atwater, and J. A. Sekorski. 1976. Refinement and Validation of an Urban Meteorological-Pollutant Model, Publication No. EPA-600/4-76-037 (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This report describes the refinement of the CEM grid model for predicting ambient concentrations. A finer (2 mile) grid was used in this study and carbon monoxide predicted concentrations in Los Angeles were compared with those made from an 8 mile grid and with ambient measurements.

Sekorski, J. A. 1976. Addendum Program Description, Publication No. EPA-600/4-76-037a (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This addendum to the above report describes the CEM computer program for the numerical grid model. Model required inputs and card format and the card deck set up are illustrated and discussed. A computer card listing of the program is given. Also, a program listing for performing statistical comparisons of model outputs is given.

Systems Applications, Inc.

Systems Applications, Inc. 1976. Continued Research in Mesoscale Air Pollution Modeling vols. I-IV, Publication No. EPA-600/4-76-016a-d (Research Triangle Park, North Carolina, U.S. Environmental Protection Agency).

This report discusses the ongoing development of the SAI photochemical model. Numerous changes from the earlier version of the model are described, including the photochemical reaction mechanism and numerical solution technique. These documents will complement a new model user's guide which will discuss in detail the computer program itself and should be available soon.

Record, F. A., R. M. Patterson, D. A. Bryant, and H. H. Castaline. 1975. *Photochemical Oxidant Modeling. Volume I: Technique Applicable to Highway System Evaluation*, Publication No. EPA-450/3-75-069a (Bedford, Mass., GCA Corporation).

This report discusses and evaluates the earlier version of the SAI model (among other models). It summarizes the various data inputs required and discusses applications and limitations of the model. Several references are provided which trace the historical development of the model and provide detailed description of it.

Regional Transport Model for Atmospheric Sulfates

Rao, S. K., I. Thomson, and B. A. Egan. 1976. "Regional Transport Model of Atmospheric Sulfates," prepared for the Electric Power Research Institute (Palo Alto, Calif., Electric Power Research Institute).

This paper describes the Regional Transport Sulfate Model developed as part of the EPRI Sulfate Regional Experiment Design Project. The model formulation and numerical solution technique are described, as are some of the model assumptions. Some of the initial comparisons of model projections with experimental data collected as part of the EPRI project are included.

Numerical Examination of Urban Smog

Sklarew, R. C., A. J. Fabrick, and J. E. Prager. 1971. *A Particle-in-Cell Method for Numerical Solution of the Atmospheric Diffusion Equation and Applications to Air Pollution Problems, Vol. 1* (La Jolla, Calif., Systems Science and Software).

This report is the companion to Volumes 2 and 3, which describe the computer code and its use. The particle-in-cell (PIC) solution technique, which was developed to alleviate the accuracy problems of other numerical solution techniques, is described and compared with other soluting techniques. The development of the NEXUS computer model, which incorporates the PIC technique, is described and model inputs and outputs are noted. An application and field validation of the NEXUS model for CO concentration predictions in Los Angeles is given. Finally, the development of a companion model, NEXUS-p, for photochemically reactive residuals is discussed.

Rollback Appendix J

Record, F. A., R. M. Patterson, D. A. Bryant, and H. H. Castaline. 1975. *Photochemical Oxidant Modeling. Volume I. Techniques Applicable to Highway System Evaluation*, Publication No. EPA-450/3-75-069a (Bedford, Mass., GCA Corporation).

This report gives a useful analysis and evaluation of the nonlinear rollback Appendix J technique. The assumptions and methodology of the technique are discussed and illustrated with the Appendix J curves. Typical model applications and the limitations of the model are given. The discussion is complemented by the previous section on linear rollback modeling.

Croke and Roberts

Mosse, H. 1970. Mathematical Urban Air Pollution Models, Publication No. ANL/ES-RPY-001 (Argonne, Illinois, Argonne National Laboratory).

This report presents the formulation of the linear regression model used by Croke and Roberts. A detailed discussion of the technique, data requirements, limitations, and interpretation is not presented, however, and the reader must consult the authors for additional information.

Repro Model

Horowitz, A., W. S. Meisel, and D. C. Collins. 1973. The Application of Repro-Modeling to the Analysis of a Photochemical Air Pollution Model (Santa Monica, Calif., Technology Service Corporation) and available as NTIS Publication No. PB 231-667.

As an alternative to the repeated application of highly complex models, this report discusses "repro modeling," the analysis and replication of model variable inputs and outputs in order to develop statistical relations between model inputs and outputs. A study of the application of repro modeling to the SAI model developed for the Los Angeles Basin is described. Examples of policy applications of the repro model are provided.